JURASSIC

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1 Main Page

The JUelich RApid Spectral SImulation Code (JURASSIC) is a fast radiative transfer model for the mid-infrared spectral region.This reference manual provides information on the algorithms and data structures used in the code.

Further information can be found at: `https://github.com/slcs-jsc/jurassic`

2 Data Structure Index

2.1 Data Structures

Here are the data structures with brief descriptions:

3 File Index

3.1 File List

Here is a list of all files with brief descriptions:

4 Data Structure Documentation

4.1 atm_t Struct Reference

Atmospheric data.

```
#include <jurassic.h>
```

Data Fields

- int np

  Number of data points.
- double time [NP]

  Time (seconds since 2000-01-01T00:00Z).
- double z [NP]

  Altitude [km].
- double lon [NP]

  Longitude [deg].
- double lat [NP]

  Latitude [deg].
- double p [NP]

  Pressure [hPa].
- double t [NP]

  Temperature [K].
- double q [NG][NP]

  Volume mixing ratio [ppv].

- double k [NW][NP]

    Extinction [1/km].
- double clz

    Cloud layer height [km].
- double cldz

    Cloud layer depth [km].
- double clk [NCL]

    Cloud layer extinction [1/km].
- double sfz

    Surface height [km].
- double sfp

    Surface pressure [hPa].
- double sft

    Surface temperature [K].
- double sfeps [NSF]

    Surface emissivity.

4.1.1 Detailed Description

Atmospheric data.

Definition at line 343 of file jurassic.h.

4.1.2 Field Documentation

4.1.2.1 np `int atm_t::np`

Number of data points.

Definition at line 346 of file jurassic.h.

4.1.2.2 time `double atm_t::time[NP]`

Time (seconds since 2000-01-01T00:00Z).

Definition at line 349 of file jurassic.h.

4.1.2.3 z `double atm_t::z[NP]`

Altitude [km].

Definition at line 352 of file jurassic.h.

4.1.2.4 lon `double atm_t::lon[NP]`

Longitude [deg].

Definition at line 355 of file jurassic.h.

4.1.2.5 lat `double atm_t::lat[NP]`

Latitude [deg].

Definition at line 358 of file jurassic.h.

4.1.2.6 p `double atm_t::p[NP]`

Pressure [hPa].

Definition at line 361 of file jurassic.h.

4.1.2.7 t `double atm_t::t[NP]`

Temperature [K].

Definition at line 364 of file jurassic.h.

4.1.2.8 q `double atm_t::q[NG][NP]`

Volume mixing ratio [ppv].

Definition at line 367 of file jurassic.h.

4.1.2.9 k `double atm_t::k[NW][NP]`

Extinction [1/km].

Definition at line 370 of file jurassic.h.

4.1.2.10 clz `double atm_t::clz`

Cloud layer height [km].

Definition at line 373 of file jurassic.h.

4.1.2.11 cldz `double atm_t::cldz`

Cloud layer depth [km].

Definition at line 376 of file jurassic.h.

4.1.2.12 clk `double atm_t::clk[NCL]`

Cloud layer extinction [1/km].

Definition at line 379 of file jurassic.h.

4.1.2.13 sfz `double atm_t::sfz`

Surface height [km].

Definition at line 382 of file jurassic.h.

4.1.2.14 sfp `double atm_t::sfp`

Surface pressure [hPa].

Definition at line 385 of file jurassic.h.

4.1.2.15 sft `double atm_t::sft`

Surface temperature [K].

Definition at line 388 of file jurassic.h.

4.1.2.16 sfeps double atm_t::sfeps[NSF]

Surface emissivity.

Definition at line 391 of file jurassic.h.

The documentation for this struct was generated from the following file:

- jurassic.h

4.2 ctl_t Struct Reference

Forward model control parameters.

```
#include <jurassic.h>
```

Data Fields

- int ng
  Number of emitters.
- char emitter [NG][LEN]
  Name of each emitter.
- int nd
  Number of radiance channels.
- double nu [ND]
  Centroid wavenumber of each channel [cm^-1].
- int nw
  Number of spectral windows.
- int window [ND]
  Window index of each channel.
- int ncl
  Number of cloud layer spectral grid points.
- double clnu [NCL]
  Cloud layer wavenumber [cm^-1].
- int nsf
  Number of surface layer spectral grid points.
- double sfnu [NSF]
  Surface layer wavenumber [cm^-1].
- int sftype
  Surface treatment (0=none, 1=emissions, 2=downward, 3=solar).
- double sfsza
  Solar zenith angle at the surface [deg] (-999=auto).
- char tblbase [LEN]
  Basename for table files and filter function files.
- int tblfmt
  Look-up table file format (1=ASCII, 2=binary).
- double hydz
  Reference height for hydrostatic pressure profile (-999 to skip) [km].
- int ctm_co2
  Compute CO2 continuum (0=no, 1=yes).

- int ctm_h2o

  Compute H2O continuum (0=no, 1=yes).
- int ctm_n2

  Compute N2 continuum (0=no, 1=yes).
- int ctm_o2

  Compute O2 continuum (0=no, 1=yes).
- int refrac

  Take into account refractivity (0=no, 1=yes).
- double rayds

  Maximum step length for raytracing [km].
- double raydz

  Vertical step length for raytracing [km].
- char fov [LEN]

  Field-of-view data file.
- double retp_zmin

  Minimum altitude for pressure retrieval [km].
- double retp_zmax

  Maximum altitude for pressure retrieval [km].
- double rett_zmin

  Minimum altitude for temperature retrieval [km].
- double rett_zmax

  Maximum altitude for temperature retrieval [km].
- double retq_zmin [NG]

  Minimum altitude for volume mixing ratio retrieval [km].
- double retq_zmax [NG]

  Maximum altitude for volume mixing ratio retrieval [km].
- double retk_zmin [NW]

  Minimum altitude for extinction retrieval [km].
- double retk_zmax [NW]

  Maximum altitude for extinction retrieval [km].
- int ret_clz

  Retrieve cloud layer height (0=no, 1=yes).
- int ret_cldz

  Retrieve cloud layer depth (0=no, 1=yes).
- int ret_clk

  Retrieve cloud layer extinction (0=no, 1=yes).
- int ret_sfz

  Retrieve surface layer height (0=no, 1=yes).
- int ret_sfp

  Retrieve surface layer pressure (0=no, 1=yes).
- int ret_sft

  Retrieve surface layer temperature (0=no, 1=yes).
- int ret_sfeps

  Retrieve surface layer emissivity (0=no, 1=yes).
- int write_bbt

  Use brightness temperature instead of radiance (0=no, 1=yes).
- int write_matrix

  Write matrix file (0=no, 1=yes).
- int formod

  Forward model (1=EGA, 2=RFM).
- char rfmbin [LEN]

Path to RFM binary.

- char rfmhit [LEN]

    HITRAN file for RFM.

- char rfmxsc [NG][LEN]

    Emitter cross-section files for RFM.

4.2.1 Detailed Description

Forward model control parameters.

Definition at line 396 of file jurassic.h.

4.2.2 Field Documentation

4.2.2.1 ng `int ctl_t::ng`

Number of emitters.

Definition at line 399 of file jurassic.h.

4.2.2.2 emitter `char ctl_t::emitter[NG][LEN]`

Name of each emitter.

Definition at line 402 of file jurassic.h.

4.2.2.3 nd `int ctl_t::nd`

Number of radiance channels.

Definition at line 405 of file jurassic.h.

4.2.2.4 nu `double ctl_t::nu[ND]`

Centroid wavenumber of each channel [cm^-1].

Definition at line 408 of file jurassic.h.

4.2.2.5 nw `int ctl_t::nw`

Number of spectral windows.

Definition at line 411 of file jurassic.h.

4.2.2.6 window `int ctl_t::window[ND]`

Window index of each channel.

Definition at line 414 of file jurassic.h.

4.2.2.7 ncl `int ctl_t::ncl`

Number of cloud layer spectral grid points.

Definition at line 417 of file jurassic.h.

4.2.2.8 clnu `double ctl_t::clnu[NCL]`

Cloud layer wavenumber [cm^-1].

Definition at line 420 of file jurassic.h.

4.2.2.9 nsf `int ctl_t::nsf`

Number of surface layer spectral grid points.

Definition at line 423 of file jurassic.h.

4.2.2.10 sfnu `double ctl_t::sfnu[NSF]`

Surface layer wavenumber [cm^-1].

Definition at line 426 of file jurassic.h.

4.2.2.11 sftype `int ctl_t::sftype`

Surface treatment (0=none, 1=emissions, 2=downward, 3=solar).

Definition at line 429 of file jurassic.h.

4.2.2.12 sfsza `double ctl_t::sfsza`

Solar zenith angle at the surface [deg] (-999=auto).

Definition at line 432 of file jurassic.h.

4.2.2.13 tblbase `char ctl_t::tblbase[LEN]`

Basename for table files and filter function files.

Definition at line 435 of file jurassic.h.

4.2.2.14 tblfmt `int ctl_t::tblfmt`

Look-up table file format (1=ASCII, 2=binary).

Definition at line 438 of file jurassic.h.

4.2.2.15 hydz `double ctl_t::hydz`

Reference height for hydrostatic pressure profile (-999 to skip) [km].

Definition at line 441 of file jurassic.h.

4.2.2.16 ctm_co2 `int ctl_t::ctm_co2`

Compute CO2 continuum (0=no, 1=yes).

Definition at line 444 of file jurassic.h.

4.2.2.17 ctm_h2o `int ctl_t::ctm_h2o`

Compute H2O continuum (0=no, 1=yes).

Definition at line 447 of file jurassic.h.

4.2.2.18 ctm_n2 `int ctl_t::ctm_n2`

Compute N2 continuum (0=no, 1=yes).

Definition at line 450 of file jurassic.h.

4.2.2.19 ctm_o2 `int ctl_t::ctm_o2`

Compute O2 continuum (0=no, 1=yes).

Definition at line 453 of file jurassic.h.

4.2.2.20 refrac `int ctl_t::refrac`

Take into account refractivity (0=no, 1=yes).

Definition at line 456 of file jurassic.h.

4.2.2.21 rayds `double ctl_t::rayds`

Maximum step length for raytracing [km].

Definition at line 459 of file jurassic.h.

4.2.2.22 raydz `double ctl_t::raydz`

Vertical step length for raytracing [km].

Definition at line 462 of file jurassic.h.

4.2.2.23 fov `char ctl_t::fov[LEN]`

Field-of-view data file.

Definition at line 465 of file jurassic.h.

4.2.2.24 retp_zmin `double ctl_t::retp_zmin`

Minimum altitude for pressure retrieval [km].

Definition at line 468 of file jurassic.h.

4.2.2.25 retp_zmax `double ctl_t::retp_zmax`

Maximum altitude for pressure retrieval [km].

Definition at line 471 of file jurassic.h.

4.2.2.26 rett_zmin `double ctl_t::rett_zmin`

Minimum altitude for temperature retrieval [km].

Definition at line 474 of file jurassic.h.

4.2.2.27 rett_zmax `double ctl_t::rett_zmax`

Maximum altitude for temperature retrieval [km].

Definition at line 477 of file jurassic.h.

4.2.2.28 retq_zmin `double ctl_t::retq_zmin[NG]`

Minimum altitude for volume mixing ratio retrieval [km].

Definition at line 480 of file jurassic.h.

4.2.2.29 retq_zmax `double ctl_t::retq_zmax[NG]`

Maximum altitude for volume mixing ratio retrieval [km].

Definition at line 483 of file jurassic.h.

4.2.2.30 retk_zmin `double ctl_t::retk_zmin[NW]`

Minimum altitude for extinction retrieval [km].

Definition at line 486 of file jurassic.h.

4.2.2.31 retk_zmax `double ctl_t::retk_zmax[NW]`

Maximum altitude for extinction retrieval [km].

Definition at line 489 of file jurassic.h.

4.2.2.32 ret_clz `int ctl_t::ret_clz`

Retrieve cloud layer height (0=no, 1=yes).

Definition at line 492 of file jurassic.h.

4.2.2.33 ret_cldz `int ctl_t::ret_cldz`

Retrieve cloud layer depth (0=no, 1=yes).

Definition at line 495 of file jurassic.h.

4.2.2.34 ret_clk `int ctl_t::ret_clk`

Retrieve cloud layer extinction (0=no, 1=yes).

Definition at line 498 of file jurassic.h.

4.2.2.35 ret_sfz `int ctl_t::ret_sfz`

Retrieve surface layer height (0=no, 1=yes).

Definition at line 501 of file jurassic.h.

4.2.2.36 ret_sfp `int ctl_t::ret_sfp`

Retrieve surface layer pressure (0=no, 1=yes).

Definition at line 504 of file jurassic.h.

4.2.2.37 ret_sft `int ctl_t::ret_sft`

Retrieve surface layer temperature (0=no, 1=yes).

Definition at line 507 of file jurassic.h.

4.2.2.38 ret_sfeps `int ctl_t::ret_sfeps`

Retrieve surface layer emissivity (0=no, 1=yes).

Definition at line 510 of file jurassic.h.

4.2.2.39 write_bbt `int ctl_t::write_bbt`

Use brightness temperature instead of radiance (0=no, 1=yes).

Definition at line 513 of file jurassic.h.

4.2.2.40 write_matrix `int ctl_t::write_matrix`

Write matrix file (0=no, 1=yes).

Definition at line 516 of file jurassic.h.

4.2.2.41 formod `int ctl_t::formod`

Forward model (1=EGA, 2=RFM).

Definition at line 519 of file jurassic.h.

4.2.2.42 rfmbin `char ctl_t::rfmbin[LEN]`

Path to RFM binary.

Definition at line 522 of file jurassic.h.

4.2.2.43 rfmhit `char ctl_t::rfmhit[LEN]`

HITRAN file for RFM.

Definition at line 525 of file jurassic.h.

4.2.2.44 rfmxsc `char ctl_t::rfmxsc[NG][LEN]`

Emitter cross-section files for RFM.

Definition at line 528 of file jurassic.h.

The documentation for this struct was generated from the following file:

- jurassic.h

4.3 los_t Struct Reference

Line-of-sight data.

```
#include <jurassic.h>
```

Data Fields

- int np
  Number of LOS points.
- double z [NLOS]
  Altitude [km].
- double lon [NLOS]
  Longitude [deg].
- double lat [NLOS]
  Latitude [deg].
- double p [NLOS]
  Pressure [hPa].
- double t [NLOS]
  Temperature [K].
- double q [NLOS][NG]
  Volume mixing ratio [ppv].
- double k [NLOS][ND]
  Extinction [1/km].
- double sft
  Surface temperature [K].
- double sfeps [ND]
  Surface emissivity.
- double ds [NLOS]
  Segment length [km].
- double u [NLOS][NG]
  Column density [molecules/cm^2].
- double eps [NLOS][ND]
  Segment emissivity.
- double src [NLOS][ND]
  Segment source function [W/(m^2 sr cm^-1)].

4.3.1 Detailed Description

Line-of-sight data.

Definition at line 533 of file jurassic.h.

4.3.2 Field Documentation

4.3.2.1 np `int los_t::np`

Number of LOS points.

Definition at line 536 of file jurassic.h.

4.3.2.2 z `double los_t::z[NLOS]`

Altitude [km].

Definition at line 539 of file jurassic.h.

4.3.2.3 lon `double los_t::lon[NLOS]`

Longitude [deg].

Definition at line 542 of file jurassic.h.

4.3.2.4 lat `double los_t::lat[NLOS]`

Latitude [deg].

Definition at line 545 of file jurassic.h.

4.3.2.5 p `double los_t::p[NLOS]`

Pressure [hPa].

Definition at line 548 of file jurassic.h.

4.3.2.6 t `double los_t::t[NLOS]`

Temperature [K].

Definition at line 551 of file jurassic.h.

4.3.2.7 q `double los_t::q[NLOS][NG]`

Volume mixing ratio [ppv].

Definition at line 554 of file jurassic.h.

4.3.2.8 k `double los_t::k[NLOS][ND]`

Extinction [1/km].

Definition at line 557 of file jurassic.h.

4.3.2.9 sft `double los_t::sft`

Surface temperature [K].

Definition at line 560 of file jurassic.h.

4.3.2.10 sfeps `double los_t::sfeps[ND]`

Surface emissivity.

Definition at line 563 of file jurassic.h.

4.3.2.11 ds `double los_t::ds[NLOS]`

Segment length [km].

Definition at line 566 of file jurassic.h.

4.3.2.12 u `double los_t::u[NLOS][NG]`

Column density [molecules/cm^2].

Definition at line 569 of file jurassic.h.

4.3.2.13 eps `double los_t::eps[NLOS][ND]`

Segment emissivity.

Definition at line 572 of file jurassic.h.

4.3.2.14 src `double los_t::src[NLOS][ND]`

Segment source function [W/(m^2 sr cm^-1)].

Definition at line 575 of file jurassic.h.

The documentation for this struct was generated from the following file:

- jurassic.h

4.4 obs_t Struct Reference

Observation geometry and radiance data.

```
#include <jurassic.h>
```

Data Fields

- int nr

  Number of ray paths.
- double time [NR]

  Time (seconds since 2000-01-01T00:00Z).
- double obsz [NR]

  Observer altitude [km].
- double obslon [NR]

  Observer longitude [deg].
- double obslat [NR]

  Observer latitude [deg].
- double vpz [NR]

  View point altitude [km].
- double vplon [NR]

  View point longitude [deg].
- double vplat [NR]

  View point latitude [deg].
- double tpz [NR]

  Tangent point altitude [km].
- double tplon [NR]

  Tangent point longitude [deg].
- double tplat [NR]

  Tangent point latitude [deg].
- double tau [ND][NR]

  Transmittance of ray path.
- double rad [ND][NR]

  Radiance [W/(m^2 sr cm^-1)].

4.4.1 Detailed Description

Observation geometry and radiance data.

Definition at line 580 of file jurassic.h.

4.4.2 Field Documentation

4.4.2.1 nr `int obs_t::nr`

Number of ray paths.

Definition at line 583 of file jurassic.h.

4.4.2.2 time `double obs_t::time[NR]`

Time (seconds since 2000-01-01T00:00Z).

Definition at line 586 of file jurassic.h.

4.4.2.3 obsz `double obs_t::obsz[NR]`

Observer altitude [km].

Definition at line 589 of file jurassic.h.

4.4.2.4 obslon `double obs_t::obslon[NR]`

Observer longitude [deg].

Definition at line 592 of file jurassic.h.

4.4.2.5 obslat `double obs_t::obslat[NR]`

Observer latitude [deg].

Definition at line 595 of file jurassic.h.

4.4.2.6 vpz `double obs_t::vpz[NR]`

View point altitude [km].

Definition at line 598 of file jurassic.h.

4.4.2.7 vplon `double obs_t::vplon[NR]`

View point longitude [deg].

Definition at line 601 of file jurassic.h.

4.4.2.8 vplat `double obs_t::vplat[NR]`

View point latitude [deg].

Definition at line 604 of file jurassic.h.

4.4.2.9 tpz `double obs_t::tpz[NR]`

Tangent point altitude [km].

Definition at line 607 of file jurassic.h.

4.4.2.10 tplon `double obs_t::tplon[NR]`

Tangent point longitude [deg].

Definition at line 610 of file jurassic.h.

4.4.2.11 tplat `double obs_t::tplat[NR]`

Tangent point latitude [deg].

Definition at line 613 of file jurassic.h.

4.4.2.12 tau `double obs_t::tau[ND][NR]`

Transmittance of ray path.

Definition at line 616 of file jurassic.h.

4.4.2.13 rad `double obs_t::rad[ND][NR]`

Radiance [W/(m^2 sr cm^-1)].

Definition at line 619 of file jurassic.h.

The documentation for this struct was generated from the following file:

- jurassic.h

4.5 ret_t Struct Reference

Retrieval control parameters.

Data Fields

- char dir [LEN]

  Working directory.
- int kernel_recomp

  Re-computation of kernel matrix (number of iterations).
- int conv_itmax

  Maximum number of iterations.
- double conv_dmin

  Minimum normalized step size in state space.
- int err_ana

  Carry out error analysis (0=no, 1=yes).
- double err_formod [ND]

  Forward model error [%].
- double err_noise [ND]

  Noise error [W/(m^2 sr cm^-1)].
- double err_press

  Pressure error [%].
- double err_press_cz

  Vertical correlation length for pressure error [km].
- double err_press_ch

  Horizontal correlation length for pressure error [km].
- double err_temp

  Temperature error [K].
- double err_temp_cz

  Vertical correlation length for temperature error [km].
- double err_temp_ch

  Horizontal correlation length for temperature error [km].
- double err_q [NG]

  Volume mixing ratio error [%].
- double err_q_cz [NG]

  Vertical correlation length for volume mixing ratio error [km].
- double err_q_ch [NG]

  Horizontal correlation length for volume mixing ratio error [km].
- double err_k [NW]

  Extinction error [1/km].

- double err_k_cz [NW]

  Vertical correlation length for extinction error [km].
- double err_k_ch [NW]

  Horizontal correlation length for extinction error [km].
- double err_clz

  Cloud height error [km].
- double err_cldz

  Cloud depth error [km].
- double err_clk [NCL]

  Cloud extinction error [1/km].
- double err_sfz

  Surface height error [km].
- double err_sfp

  Surface pressure error [hPa].
- double err_sft

  Surface temperature error [K].
- double err_sfeps [NSF]

  Surface emissivity error.

4.5.1 Detailed Description

Retrieval control parameters.

Definition at line 32 of file retrieval.c.

4.5.2 Field Documentation

4.5.2.1 dir `char ret_t::dir[LEN]`

Working directory.

Definition at line 35 of file retrieval.c.

4.5.2.2 kernel_recomp `int ret_t::kernel_recomp`

Re-computation of kernel matrix (number of iterations).

Definition at line 38 of file retrieval.c.

4.5.2.3 conv_itmax `int ret_t::conv_itmax`

Maximum number of iterations.

Definition at line 41 of file retrieval.c.

4.5.2.4 conv_dmin `double ret_t::conv_dmin`

Minimum normalized step size in state space.

Definition at line 44 of file retrieval.c.

4.5.2.5 err_ana `int ret_t::err_ana`

Carry out error analysis (0=no, 1=yes).

Definition at line 47 of file retrieval.c.

4.5.2.6 err_formod `double ret_t::err_formod[ND]`

Forward model error [%].

Definition at line 50 of file retrieval.c.

4.5.2.7 err_noise `double ret_t::err_noise[ND]`

Noise error [W/(m^2 sr cm^-1)].

Definition at line 53 of file retrieval.c.

4.5.2.8 err_press `double ret_t::err_press`

Pressure error [%].

Definition at line 56 of file retrieval.c.

4.5.2.9 err_press_cz `double ret_t::err_press_cz`

Vertical correlation length for pressure error [km].

Definition at line 59 of file retrieval.c.

4.5.2.10 err_press_ch `double ret_t::err_press_ch`

Horizontal correlation length for pressure error [km].

Definition at line 62 of file retrieval.c.

4.5.2.11 err_temp `double ret_t::err_temp`

Temperature error [K].

Definition at line 65 of file retrieval.c.

4.5.2.12 err_temp_cz `double ret_t::err_temp_cz`

Vertical correlation length for temperature error [km].

Definition at line 68 of file retrieval.c.

4.5.2.13 err_temp_ch `double ret_t::err_temp_ch`

Horizontal correlation length for temperature error [km].

Definition at line 71 of file retrieval.c.

4.5.2.14 err_q `double ret_t::err_q[NG]`

Volume mixing ratio error [%].

Definition at line 74 of file retrieval.c.

4.5.2.15 err_q_cz `double ret_t::err_q_cz[NG]`

Vertical correlation length for volume mixing ratio error [km].

Definition at line 77 of file retrieval.c.

4.5.2.16 err_q_ch `double ret_t::err_q_ch[NG]`

Horizontal correlation length for volume mixing ratio error [km].

Definition at line 80 of file retrieval.c.

4.5.2.17 err_k `double ret_t::err_k[NW]`

Extinction error [1/km].

Definition at line 83 of file retrieval.c.

4.5.2.18 err_k_cz `double ret_t::err_k_cz[NW]`

Vertical correlation length for extinction error [km].

Definition at line 86 of file retrieval.c.

4.5.2.19 err_k_ch `double ret_t::err_k_ch[NW]`

Horizontal correlation length for extinction error [km].

Definition at line 89 of file retrieval.c.

4.5.2.20 err_clz `double ret_t::err_clz`

Cloud height error [km].

Definition at line 92 of file retrieval.c.

4.5.2.21 err_cldz `double ret_t::err_cldz`

Cloud depth error [km].

Definition at line 95 of file retrieval.c.

4.5.2.22 err_clk `double ret_t::err_clk[NCL]`

Cloud extinction error [1/km].

Definition at line 98 of file retrieval.c.

4.5.2.23 err_sfz `double ret_t::err_sfz`

Surface height error [km].

Definition at line 101 of file retrieval.c.

4.5.2.24 err_sfp `double ret_t::err_sfp`

Surface pressure error [hPa].

Definition at line 104 of file retrieval.c.

4.5.2.25 err_sft `double ret_t::err_sft`

Surface temperature error [K].

Definition at line 107 of file retrieval.c.

4.5.2.26 err_sfeps `double ret_t::err_sfeps[NSF]`

Surface emissivity error.

Definition at line 110 of file retrieval.c.

The documentation for this struct was generated from the following file:

- retrieval.c

4.6 tbl_t Struct Reference

Emissivity look-up tables.

```
#include <jurassic.h>
```

Data Fields

- int np [ND][NG]

  Number of pressure levels.
- int nt [ND][NG][TBLNP]

  Number of temperatures.
- int nu [ND][NG][TBLNP][TBLNT]

  Number of column densities.
- double p [ND][NG][TBLNP]

  Pressure [hPa].
- double t [ND][NG][TBLNP][TBLNT]

  Temperature [K].
- float u [ND][NG][TBLNP][TBLNT][TBLNU]

  Column density [molecules/cm^2].
- float eps [ND][NG][TBLNP][TBLNT][TBLNU]

  Emissivity.
- double st [TBLNS]

  Source function temperature [K].
- double sr [TBLNS][ND]

  Source function radiance [W/(m^2 sr cm^-1)].

4.6.1 Detailed Description

Emissivity look-up tables.

Definition at line 624 of file jurassic.h.

4.6.2 Field Documentation

4.6.2.1 np `int tbl_t::np[ND][NG]`

Number of pressure levels.

Definition at line 627 of file jurassic.h.

4.6.2.2 nt `int tbl_t::nt[ND][NG][TBLNP]`

Number of temperatures.

Definition at line 630 of file jurassic.h.

4.6.2.3 nu `int tbl_t::nu[ND][NG][TBLNP][TBLNT]`

Number of column densities.

Definition at line 633 of file jurassic.h.

4.6.2.4 p `double tbl_t::p[ND][NG][TBLNP]`

Pressure [hPa].

Definition at line 636 of file jurassic.h.

4.6.2.5 t `double tbl_t::t[ND][NG][TBLNP][TBLNT]`

Temperature [K].

Definition at line 639 of file jurassic.h.

4.6.2.6 u `float tbl_t::u[ND][NG][TBLNP][TBLNT][TBLNU]`

Column density [molecules/cm^2].

Definition at line 642 of file jurassic.h.

4.6.2.7 eps `float tbl_t::eps[ND][NG][TBLNP][TBLNT][TBLNU]`

Emissivity.

Definition at line 645 of file jurassic.h.

4.6.2.8 st `double tbl_t::st[TBLNS]`

Source function temperature [K].

Definition at line 648 of file jurassic.h.

4.6.2.9 sr `double tbl_t::sr[TBLNS][ND]`

Source function radiance [W/(m^2 sr cm^-1)].

Definition at line 651 of file jurassic.h.

The documentation for this struct was generated from the following file:

- jurassic.h

5 File Documentation

5.1 brightness.c File Reference

Convert radiance to brightness temperature.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.1.1 Detailed Description

Convert radiance to brightness temperature.

Definition in file brightness.c.

5.1.2 Function Documentation

5.1.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file brightness.c.

```
                  {

  /* Check arguments... */
  if (argc != 3 && argc != 7)
    ERRMSG
      ("Give parameters: [ <rad> <nu> | "
       " <rad0> <rad1> <drad> <nu0> <nu1> <dnu> ]");

  /* Calculate single value... */
  if (argc == 3) {

    /* Read arguments... */
    double rad = atof(argv[1]);
    double nu = atof(argv[2]);

    /* Compute brightness temperature... */
    printf("%.10g\n", brightness(rad, nu));

  }

  /* Calculate table... */
  else if (argc == 7) {

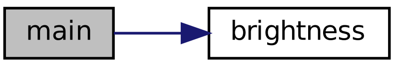
    /* Read arguments... */
    double rad0 = atof(argv[1]);
    double rad1 = atof(argv[2]);
    double drad = atof(argv[3]);
    double nu0 = atof(argv[4]);
    double nu1 = atof(argv[5]);
    double dnu = atof(argv[6]);

    /* Write header... */
    printf("# $1 = radiance [W/(m^2 sr cm^-1)]\n"
           "# $2 = wavenumber [cm^-1]\n"
           "# $3 = brightness temperature [K]\n");

    /* Compute brightness temperature... */
    for (double rad = rad0; rad <= rad1; rad += drad) {
      printf("\n");
      for (double nu = nu0; nu <= nu1; nu += dnu)
        printf("%.10g %.4f %.10g\n", rad, nu, brightness(rad, nu));
    }
  }

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.2 brightness.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
```

```
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  /* Check arguments... */
  if (argc != 3 && argc != 7)
    ERRMSG
      ("Give parameters: [ <rad> <nu> | "
       " <rad0> <rad1> <drad> <nu0> <nu1> <dnu> ]");

  /* Calculate single value... */
  if (argc == 3) {

    /* Read arguments... */
    double rad = atof(argv[1]);
    double nu = atof(argv[2]);

    /* Compute brightness temperature... */
    printf("%.10g\n", brightness(rad, nu));

  }

  /* Calculate table... */
  else if (argc == 7) {

    /* Read arguments... */
    double rad0 = atof(argv[1]);
    double rad1 = atof(argv[2]);
    double drad = atof(argv[3]);
    double nu0 = atof(argv[4]);
    double nu1 = atof(argv[5]);
    double dnu = atof(argv[6]);

    /* Write header... */
    printf("# $1 = radiance [W/(m^2 sr cm^-1)]\n"
           "# $2 = wavenumber [cm^-1]\n"
           "# $3 = brightness temperature [K]\n");

    /* Compute brightness temperature... */
    for (double rad = rad0; rad <= rad1; rad += drad) {
      printf("\n");
      for (double nu = nu0; nu <= nu1; nu += dnu)
        printf("%.10g %.4f %.10g\n", rad, nu, brightness(rad, nu));
    }
  }

  return EXIT_SUCCESS;
}
```

5.3 climatology.c File Reference

Prepare atmospheric data file from climatological data.

`#include "jurassic.h"`

Functions

- int main (int argc, char *argv[ ])

5.3.1 Detailed Description

Prepare atmospheric data file from climatological data.

Definition in file climatology.c.

5.3.2 Function Documentation

5.3.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file climatology.c.

```
                      {

  static atm_t atm;
  static ctl_t ctl;

  double clk[NCL], sfeps[NSF];

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <atm>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  double t0 = scan_ctl(argc, argv, "T0", -1, "0", NULL);
  double t1 = scan_ctl(argc, argv, "T1", -1, "0", NULL);
  double dt = scan_ctl(argc, argv, "DT", -1, "1", NULL);
  double z0 = scan_ctl(argc, argv, "Z0", -1, "0", NULL);
  double z1 = scan_ctl(argc, argv, "Z1", -1, "90", NULL);
  double dz = scan_ctl(argc, argv, "DZ", -1, "1", NULL);
  double clz = scan_ctl(argc, argv, "CLZ", -1, "0", NULL);
  double cldz = scan_ctl(argc, argv, "CLDZ", -1, "0", NULL);
  for (int icl = 0; icl < ctl.ncl; icl++)
    clk[icl] = scan_ctl(argc, argv, "CLK", icl, "0", NULL);
  double sfz = scan_ctl(argc, argv, "SFZ", -1, "0", NULL);
  double sfp = scan_ctl(argc, argv, "SFP", -1, "0", NULL);
  double sft = scan_ctl(argc, argv, "SFT", -1, "0", NULL);
  for (int isf = 0; isf < ctl.nsf; isf++)
    sfeps[isf] = scan_ctl(argc, argv, "SFEPS", isf, "1", NULL);

  /* Set atmospheric grid... */
  for (double t = t0; t <= t1; t += dt)
    for (double z = z0; z <= z1; z += dz) {
      atm.time[atm.np] = t;
      atm.z[atm.np] = z;
      if ((++atm.np) >= NP)
        ERRMSG("Too many atmospheric grid points!");
    }

  /* Interpolate climatological data... */
  climatology(&ctl, &atm);

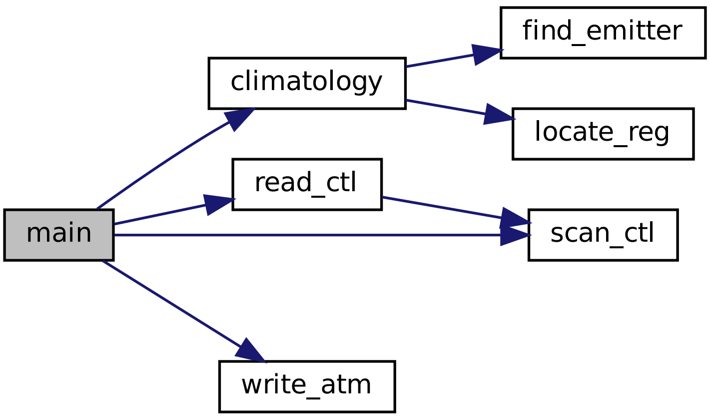
  /* Set cloud layer... */
  atm.clz = clz;
  atm.cldz = cldz;
  for (int icl = 0; icl < ctl.ncl; icl++)
    atm.clk[icl] = clk[icl];

  /* Set surface layer... */
  atm.sfz = sfz;
  atm.sfp = sfp;
  atm.sft = sft;
  for (int isf = 0; isf < ctl.nsf; isf++)
    atm.sfeps[isf] = sfeps[isf];

  /* Write data to disk... */
  write_atm(NULL, argv[2], &ctl, &atm);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.4 climatology.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static atm_t atm;
  static ctl_t ctl;

  double clk[NCL], sfeps[NSF];

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <atm>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  double t0 = scan_ctl(argc, argv, "T0", -1, "0", NULL);
  double t1 = scan_ctl(argc, argv, "T1", -1, "0", NULL);
  double dt = scan_ctl(argc, argv, "DT", -1, "1", NULL);
  double z0 = scan_ctl(argc, argv, "Z0", -1, "0", NULL);
  double z1 = scan_ctl(argc, argv, "Z1", -1, "90", NULL);
  double dz = scan_ctl(argc, argv, "DZ", -1, "1", NULL);
  double clz = scan_ctl(argc, argv, "CLZ", -1, "0", NULL);
  double cldz = scan_ctl(argc, argv, "CLDZ", -1, "0", NULL);
  for (int icl = 0; icl < ctl.ncl; icl++)
    clk[icl] = scan_ctl(argc, argv, "CLK", icl, "0", NULL);
  double sfz = scan_ctl(argc, argv, "SFZ", -1, "0", NULL);
  double sfp = scan_ctl(argc, argv, "SFP", -1, "0", NULL);
```

```
  double sft = scan_ctl(argc, argv, "SFT", -1, "0", NULL);
  for (int isf = 0; isf < ctl.nsf; isf++)
    sfeps[isf] = scan_ctl(argc, argv, "SFEPS", isf, "1", NULL);

  /* Set atmospheric grid... */
  for (double t = t0; t <= t1; t += dt)
    for (double z = z0; z <= z1; z += dz) {
      atm.time[atm.np] = t;
      atm.z[atm.np] = z;
      if ((++atm.np) >= NP)
        ERRMSG("Too many atmospheric grid points!");
    }

  /* Interpolate climatological data... */
  climatology(&ctl, &atm);

  /* Set cloud layer... */
  atm.clz = clz;
  atm.cldz = cldz;
  for (int icl = 0; icl < ctl.ncl; icl++)
    atm.clk[icl] = clk[icl];

  /* Set surface layer... */
  atm.sfz = sfz;
  atm.sfp = sfp;
  atm.sft = sft;
  for (int isf = 0; isf < ctl.nsf; isf++)
    atm.sfeps[isf] = sfeps[isf];

  /* Write data to disk... */
  write_atm(NULL, argv[2], &ctl, &atm);

  return EXIT_SUCCESS;
}
```

5.5 filter.c File Reference

Create radiometric filter functions.

```
#include "jurassic.h"
```

Functions

- double ails (int apo, double opl, double dnu)

  Compute apodized instrument line shape.
- int main (int argc, char *argv[ ])

5.5.1 Detailed Description

Create radiometric filter functions.

Definition in file filter.c.

5.5.2 Function Documentation

5.5.2.1 ails()

```
double ails (
    int apo,
    double opl,
    double dnu )
```

Compute apodized instrument line shape.

Definition at line 120 of file filter.c.

```
{

  double a, a2, a4, a6, a8, cosa, q0, q2, q4, sinca;

  /* Auxiliary quantities... */
  a = 2 * M_PI * dnu * opl;
  a2 = a * a;
  a4 = a2 * a2;
  a6 = a4 * a2;
  a8 = a4 * a4;

  /* Sinc function... */
  if (apo == 0) {
    if (fabs(a) < 0.7)
      return 1 - a2 / 6 + a4 / 120 - a6 / 5040 + a8 / 362880;
    else
      return sin(a) / a;
  }

  /* Norton-Beer strong apodization... */
  else if (apo == 1) {
    if (fabs(a) < 0.7) {
      q0 = 1 - a2 / 6 + a4 / 120 - a6 / 5040 + a8 / 362880;
      q2 = 1 - a2 / 14 + a4 / 504 - a6 / 33264 + a8 / 3459456;
      q4 = 1 - a2 / 22 + a4 / 1144 - a6 / 102960 + a8 / 14002560;
    } else {
      sinca = sin(a) / a;
      cosa = cos(a);
      q0 = sinca;
      q2 = -15 / a2 * ((1 - 3 / a2) * sinca + (3 / a2) * cosa);
      q4 =
        945 / a4 * ((1 - 45 / a2 + 105 / a4) * sinca +
                    5 / a2 * (2 - 21 / a2) * cosa);
    }
    return 0.045335 * q0 + 0.554883 * q2 * 8. / 15. +
      0.399782 * q4 * 384. / 945.;
  }

  /* Error message.... */
  else
    ERRMSG("Unknown apodization!");
}
```

5.5.2.2 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 41 of file filter.c.

```
{

  static ctl_t ctl;

  static double ff[NSHAPE], fnu[NSHAPE];

  double fsum = 0.0;

  int fn = 0;

  /* Write info... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <filter>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  int type = (int) scan_ctl(argc, argv, "FILTER_TYPE", -1, "1", NULL);
  double opd = scan_ctl(argc, argv, "FILTER_OPD", -1, "10.0", NULL);
  double fwhm = scan_ctl(argc, argv, "FILTER_FWHM", -1, "1.0", NULL);
  double center = scan_ctl(argc, argv, "FILTER_CENTER", -1, "1000.0", NULL);
```

```
  double width = scan_ctl(argc, argv, "FILTER_WIDTH", -1, "2.1", NULL);
  double samp = scan_ctl(argc, argv, "FILTER_SAMP", -1, "0.0005", NULL);

  /* Compute filter function... */
  for (double nu = center - 0.5 * width;
       nu <= center + 0.5 * width; nu += samp) {

    /* Set frequency... */
    fnu[fn] = nu;

    /* Boxcar... */
    if (type == 0)
      ff[fn] = (fabs(nu - center) <= 0.5 * fwhm ? 1.0 : 0.0);

    /* Triangle... */
    else if (type == 1) {
      ff[fn] = 1.0 - fabs(nu - center) / fwhm;
      ff[fn] = GSL_MAX(ff[fn], 0.0);
    }

    /* Gaussian... */
    else if (type == 2) {
      double sigma = fwhm / 2.355;
      ff[fn] = exp(-0.5 * POW2((nu - center) / sigma));
    }

    /* Sinc function... */
    else if (type == 3)
      ff[fn] = ails(0, opd, nu - center);

    /* Norton-Beer strong apodization... */
    else if (type == 4)
      ff[fn] = ails(1, opd, nu - center);

    /* Error message... */
    else
      ERRMSG("Filter function type unknown!");

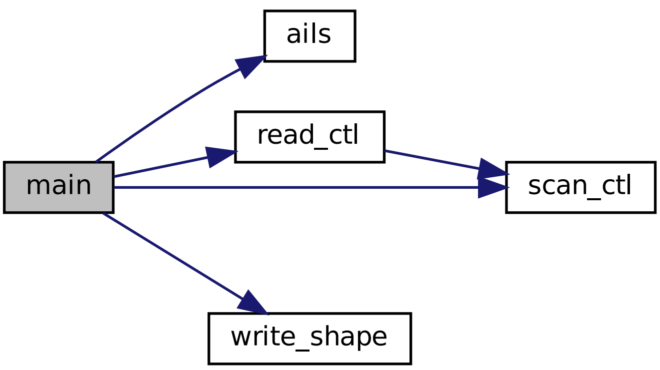
    /* Count spectral grid points... */
    if ((++fn) >= NSHAPE)
      ERRMSG("Too many filter function data points!");
  }

  /* Normalize filter function... */
  for (int i = 0; i < fn; i++)
    fsum += ff[i];
  for (int i = 0; i < fn; i++)
    ff[i] /= (fsum * samp);

  /* Write to file... */
  write_shape(argv[2], fnu, ff, fn);

  return (EXIT_SUCCESS);
}
```

Here is the call graph for this function:



5.6 filter.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

/* ------------------------------------------------------------
   Functions...
   ------------------------------------------------------------ */

double ails(
  int apo,
  double opl,
  double dnu);

/* ------------------------------------------------------------
   Main...
   ------------------------------------------------------------ */

int main(
  int argc,
  char *argv[]) {

  static ctl_t ctl;

  static double ff[NSHAPE], fnu[NSHAPE];

  double fsum = 0.0;

  int fn = 0;

  /* Write info... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <filter>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  int type = (int) scan_ctl(argc, argv, "FILTER_TYPE", -1, "1", NULL);
  double opd = scan_ctl(argc, argv, "FILTER_OPD", -1, "10.0", NULL);
  double fwhm = scan_ctl(argc, argv, "FILTER_FWHM", -1, "1.0", NULL);
  double center = scan_ctl(argc, argv, "FILTER_CENTER", -1, "1000.0", NULL);
  double width = scan_ctl(argc, argv, "FILTER_WIDTH", -1, "2.1", NULL);
  double samp = scan_ctl(argc, argv, "FILTER_SAMP", -1, "0.0005", NULL);

  /* Compute filter function... */
  for (double nu = center - 0.5 * width;
       nu <= center + 0.5 * width; nu += samp) {

    /* Set frequency... */
    fnu[fn] = nu;

    /* Boxcar... */
    if (type == 0)
      ff[fn] = (fabs(nu - center) <= 0.5 * fwhm ? 1.0 : 0.0);

    /* Triangle... */
    else if (type == 1) {
      ff[fn] = 1.0 - fabs(nu - center) / fwhm;
      ff[fn] = GSL_MAX(ff[fn], 0.0);
    }

    /* Gaussian... */
    else if (type == 2) {
      double sigma = fwhm / 2.355;
      ff[fn] = exp(-0.5 * POW2((nu - center) / sigma));
    }

    /* Sinc function... */
    else if (type == 3)
      ff[fn] = ails(0, opd, nu - center);
```

```
    /* Norton-Beer strong apodization... */
    else if (type == 4)
      ff[fn] = ails(1, opd, nu - center);

    /* Error message... */
    else
      ERRMSG("Filter function type unknown!");

    /* Count spectral grid points... */
    if ((++fn) >= NSHAPE)
      ERRMSG("Too many filter function data points!");
  }

  /* Normalize filter function... */
  for (int i = 0; i < fn; i++)
    fsum += ff[i];
  for (int i = 0; i < fn; i++)
    ff[i] /= (fsum * samp);

  /* Write to file... */
  write_shape(argv[2], fnu, ff, fn);

  return (EXIT_SUCCESS);
}

/*****************************************************************************/

double ails(
  int apo,
  double opl,
  double dnu) {

  double a, a2, a4, a6, a8, cosa, q0, q2, q4, sinca;

  /* Auxiliary quantities... */
  a = 2 * M_PI * dnu * opl;
  a2 = a * a;
  a4 = a2 * a2;
  a6 = a4 * a2;
  a8 = a4 * a4;

  /* Sinc function... */
  if (apo == 0) {
    if (fabs(a) < 0.7)
      return 1 - a2 / 6 + a4 / 120 - a6 / 5040 + a8 / 362880;
    else
      return sin(a) / a;
  }

  /* Norton-Beer strong apodization... */
  else if (apo == 1) {
    if (fabs(a) < 0.7) {
      q0 = 1 - a2 / 6 + a4 / 120 - a6 / 5040 + a8 / 362880;
      q2 = 1 - a2 / 14 + a4 / 504 - a6 / 33264 + a8 / 3459456;
      q4 = 1 - a2 / 22 + a4 / 1144 - a6 / 102960 + a8 / 14002560;
    } else {
      sinca = sin(a) / a;
      cosa = cos(a);
      q0 = sinca;
      q2 = -15 / a2 * ((1 - 3 / a2) * sinca + (3 / a2) * cosa);
      q4 =
        945 / a4 * ((1 - 45 / a2 + 105 / a4) * sinca +
                    5 / a2 * (2 - 21 / a2) * cosa);
    }
    return 0.045335 * q0 + 0.554883 * q2 * 8. / 15. +
      0.399782 * q4 * 384. / 945.;
  }

  /* Error message.... */
  else
    ERRMSG("Unknown apodization!");
}
```

5.7 formod.c File Reference

JURASSIC forward model.

```
#include "jurassic.h"
```

Functions

- void call_formod (ctl_t *ctl, const char *wrkdir, const char *obsfile, const char *atmfile, const char *radfile, const char *task)

  Perform forward model calculations in a single directory.
- int main (int argc, char *argv[ ])

5.7.1 Detailed Description

JURASSIC forward model.

Definition in file formod.c.

5.7.2 Function Documentation

5.7.2.1 call_formod()

```
void call_formod (
        ctl_t * ctl,
        const char * wrkdir,
        const char * obsfile,
        const char * atmfile,
        const char * radfile,
        const char * task )
```

Perform forward model calculations in a single directory.

Definition at line 122 of file formod.c.

```
                      {

  static atm_t atm, atm2;
  static obs_t obs, obs2;

  char filename[LEN];

  /* Read observation geometry... */
  read_obs(wrkdir, obsfile, ctl, &obs);

  /* Read atmospheric data... */
  read_atm(wrkdir, atmfile, ctl, &atm);

  /* Compute multiple profiles... */
  if (task[0] == 'p' || task[0] == 'P') {

    /* Loop over ray paths... */
    for (int ir = 0; ir < obs.nr; ir++) {

      /* Get atmospheric data... */
      atm2.np = 0;
      for (int ip = 0; ip < atm.np; ip++)
        if (atm.time[ip] == obs.time[ir]) {
          atm2.time[atm2.np] = atm.time[ip];
          atm2.z[atm2.np] = atm.z[ip];
          atm2.lon[atm2.np] = atm.lon[ip];
          atm2.lat[atm2.np] = atm.lat[ip];
          atm2.p[atm2.np] = atm.p[ip];
          atm2.t[atm2.np] = atm.t[ip];
          for (int ig = 0; ig < ctl->ng; ig++)
            atm2.q[ig][atm2.np] = atm.q[ig][ip];
          for (int iw = 0; iw < ctl->nw; iw++)
            atm2.k[iw][atm2.np] = atm.k[iw][ip];
          atm2.np++;
        }

      /* Get observation data... */
      obs2.nr = 1;
```

```
      obs2.time[0] = obs.time[ir];
      obs2.vpz[0] = obs.vpz[ir];
      obs2.vplon[0] = obs.vplon[ir];
      obs2.vplat[0] = obs.vplat[ir];
      obs2.obsz[0] = obs.obsz[ir];
      obs2.obslon[0] = obs.obslon[ir];
      obs2.obslat[0] = obs.obslat[ir];

      /* Check number of data points... */
      if (atm2.np > 0) {

        /* Call forward model... */
        formod(ctl, &atm2, &obs2);

        /* Save radiance data... */
        for (int id = 0; id < ctl->nd; id++) {
          obs.rad[id][ir] = obs2.rad[id][0];
          obs.tau[id][ir] = obs2.tau[id][0];
        }
      }
    }

    /* Write radiance data... */
    write_obs(wrkdir, radfile, ctl, &obs);
  }

  /* Compute single profile... */
  else {

    /* Call forward model... */
    formod(ctl, &atm, &obs);

    /* Save radiance data... */
    write_obs(wrkdir, radfile, ctl, &obs);

    /* Compute contributions... */
    if (task[0] == 'c' || task[0] == 'C') {

      /* Switch off continua... */
      ctl->ctm_co2 = 0;
      ctl->ctm_h2o = 0;
      ctl->ctm_n2 = 0;
      ctl->ctm_o2 = 0;

      /* Loop over emitters... */
      for (int ig = 0; ig < ctl->ng; ig++) {

        /* Copy atmospheric data... */
        copy_atm(ctl, &atm2, &atm, 0);

        /* Set extinction to zero... */
        for (int iw = 0; iw < ctl->nw; iw++)
          for (int ip = 0; ip < atm2.np; ip++)
            atm2.k[iw][ip] = 0;

        /* Set volume mixing ratios to zero... */
        for (int ig2 = 0; ig2 < ctl->ng; ig2++)
          if (ig2 != ig)
            for (int ip = 0; ip < atm2.np; ip++)
              atm2.q[ig2][ip] = 0;

        /* Call forward model... */
        formod(ctl, &atm2, &obs);

        /* Save radiance data... */
        sprintf(filename, "%s.%s", radfile, ctl->emitter[ig]);
        write_obs(wrkdir, filename, ctl, &obs);
      }

      /* Copy atmospheric data... */
      copy_atm(ctl, &atm2, &atm, 0);

      /* Set volume mixing ratios to zero... */
      for (int ig = 0; ig < ctl->ng; ig++)
        for (int ip = 0; ip < atm2.np; ip++)
          atm2.q[ig][ip] = 0;

      /* Call forward model... */
      formod(ctl, &atm2, &obs);

      /* Save radiance data... */
      sprintf(filename, "%s.EXTINCT", radfile);
      write_obs(wrkdir, filename, ctl, &obs);
    }

    /* Measure CPU-time... */
    if (task[0] == 't' || task[0] == 'T') {
```

```
    /* Init... */
    double t_min, t_max, t_mean = 0, t_sigma = 0;
    int n = 0;

    /* Initialize random number generator... */
    gsl_rng_env_setup();
    gsl_rng *rng = gsl_rng_alloc(gsl_rng_default);

    /* Loop over profiles... */
    do {

      /* Create random atmosphere... */
      copy_atm(ctl, &atm2, &atm, 0);
      double dtemp = 40. * (gsl_rng_uniform(rng) - 0.5);
      double dpress = 1. - 0.1 * gsl_rng_uniform(rng);
      double dq[NG];
      for (int ig = 0; ig < ctl->ng; ig++)
        dq[ig] = 0.8 + 0.4 * gsl_rng_uniform(rng);
      for (int ip = 0; ip < atm2.np; ip++) {
        atm.t[ip] += dtemp;
        atm.p[ip] *= dpress;
        for (int ig = 0; ig < ctl->ng; ig++)
          atm.q[ig][ip] *= dq[ig];
      }

      /* Measure runtime... */
      double t0 = omp_get_wtime();
      formod(ctl, &atm2, &obs);
      double dt = omp_get_wtime() - t0;

      /* Get runtime statistics... */
      t_mean += (dt);
      t_sigma += POW2(dt);
      if (n == 0 || dt < t_min)
        t_min = dt;
      if (n == 0 || dt > t_max)
        t_max = dt;
      n++;

    } while (t_mean < 10.0);

    /* Write results... */
    t_mean /= (double) n;
    t_sigma = sqrt(t_sigma / (double) n - POW2(t_mean));
    printf("RUNTIME_MEAN = %g s\n", t_mean);
    printf("RUNTIME_SIGMA = %g s\n", t_sigma);
    printf("RUNTIME_MIN = %g s\n", t_min);
    printf("RUNTIME_MAX = %g s\n", t_max);
    printf("RAYS_PER_SECOND = %g", (double) obs.nr / t_mean);
  }

  /* Analyze effect of step size... */
  if (task[0] == 's' || task[0] == 'S') {

    /* Reference run... */
    ctl->rayds = 0.1;
    ctl->raydz = 0.01;
    formod(ctl, &atm, &obs);
    copy_obs(ctl, &obs2, &obs, 0);

    /* Loop over step size... */
    for (double dz = 0.01; dz <= 2; dz *= 1.1) {
      printf("STEPSIZE: \n");
      for (double ds = 0.1; ds <= 50; ds *= 1.1) {

        /* Set step size... */
        ctl->rayds = ds;
        ctl->raydz = dz;

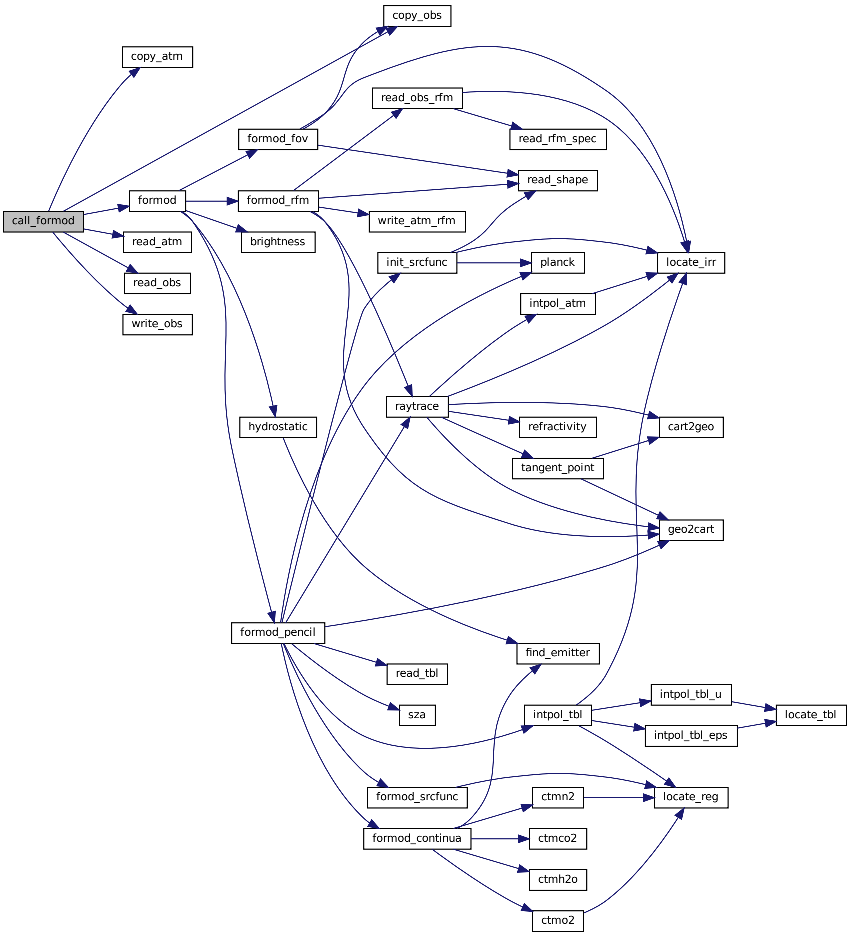
        /* Measure runtime... */
        double t0 = omp_get_wtime();
        formod(ctl, &atm, &obs);
        double dt = omp_get_wtime() - t0;

        /* Get differences... */
        double mean[ND], sigma[ND];
        for (int id = 0; id < ctl->nd; id++) {
          mean[id] = sigma[id] = 0;
          int n = 0;
          for (int ir = 0; ir < obs.nr; ir++) {
            double err = 200. * (obs.rad[id][ir] - obs2.rad[id][ir])
              / (obs.rad[id][ir] + obs2.rad[id][ir]);
            mean[id] += err;
            sigma[id] += POW2(err);
            n++;
          }
```

```
            mean[id] /= n;
            sigma[id] = sqrt(sigma[id] / n - POW2(mean[id]));
          }

          /* Write results... */
          printf("STEPSIZE: %g %g %g", ds, dz, dt);
          for (int id = 0; id < ctl->nd; id++)
            printf(" %g %g", mean[id], sigma[id]);
          printf("\n");
        }
      }
    }
  }
}
```

Here is the call graph for this function:



5.7.2.2 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 47 of file formod.c.

```
{

  static ctl_t ctl;

```

```
  /* Check arguments... */
  if (argc < 5)
    ERRMSG("Give parameters: <ctl> <obs> <atm> <rad>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

#ifdef UNIFIED

  static atm_t atm;
  static obs_t obs;

  /* Read observation geometry... */
  read_obs(NULL, argv[2], &ctl, &obs);

  /* Read atmospheric data... */
  read_atm(NULL, argv[3], &ctl, &atm);

  /* Call forward model... */
  jur_unified_init(argc, argv);
  jur_unified_formod_multiple_packages(&atm, &obs, 1, NULL);

  /* Save radiance data... */
  write_obs(NULL, argv[4], &ctl, &obs);

#else

  FILE *in;

  char dirlist[LEN], task[LEN], wrkdir[LEN];

  /* Get task... */
  scan_ctl(argc, argv, "TASK", -1, "-", task);

  /* Get dirlist... */
  scan_ctl(argc, argv, "DIRLIST", -1, "-", dirlist);

  /* Single forward calculation... */
  if (dirlist[0] == '-')
    call_formod(&ctl, NULL, argv[2], argv[3], argv[4], task);

  /* Work on directory list... */
  else {

    /* Open directory list... */
    if (!(in = fopen(dirlist, "r")))
      ERRMSG("Cannot open directory list!");

    /* Loop over directories... */
    while (fscanf(in, "%s", wrkdir) != EOF) {

      /* Write info... */
      LOG(1, "\nWorking directory: %s", wrkdir);

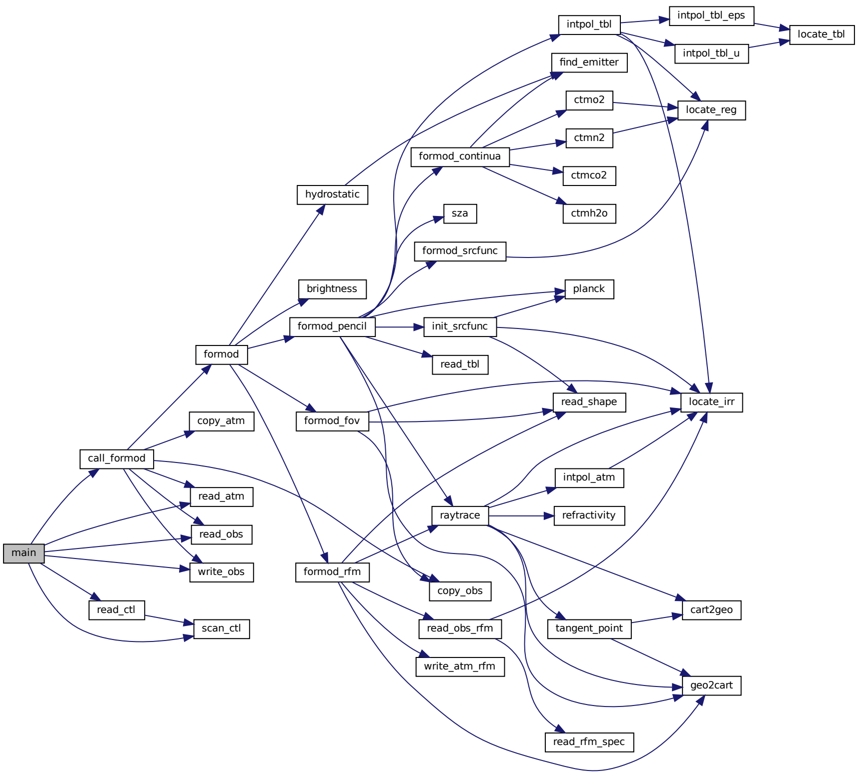
      /* Call forward model... */
      call_formod(&ctl, wrkdir, argv[2], argv[3], argv[4], task);
    }

    /* Close dirlist... */
    fclose(in);
  }

#endif

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.8 formod.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"
#ifdef UNIFIED
#include "jurassic_unified_library.h"
#endif

/* ------------------------------------------------------------
   Functions...
   ------------------------------------------------------------ */

void call_formod(
  ctl_t * ctl,
  const char *wrkdir,
  const char *obsfile,
  const char *atmfile,
  const char *radfile,
  const char *task);

/* ------------------------------------------------------------
   Main...
```

```
   ------------------------------------------------------------ */

int main(
  int argc,
  char *argv[]) {

  static ctl_t ctl;

  /* Check arguments... */
  if (argc < 5)
    ERRMSG("Give parameters: <ctl> <obs> <atm> <rad>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

#ifdef UNIFIED

  static atm_t atm;
  static obs_t obs;

  /* Read observation geometry... */
  read_obs(NULL, argv[2], &ctl, &obs);

  /* Read atmospheric data... */
  read_atm(NULL, argv[3], &ctl, &atm);

  /* Call forward model... */
  jur_unified_init(argc, argv);
  jur_unified_formod_multiple_packages(&atm, &obs, 1, NULL);

  /* Save radiance data... */
  write_obs(NULL, argv[4], &ctl, &obs);

#else

  FILE *in;

  char dirlist[LEN], task[LEN], wrkdir[LEN];

  /* Get task... */
  scan_ctl(argc, argv, "TASK", -1, "-", task);

  /* Get dirlist... */
  scan_ctl(argc, argv, "DIRLIST", -1, "-", dirlist);

  /* Single forward calculation... */
  if (dirlist[0] == '-')
    call_formod(&ctl, NULL, argv[2], argv[3], argv[4], task);

  /* Work on directory list... */
  else {

    /* Open directory list... */
    if (!(in = fopen(dirlist, "r")))
      ERRMSG("Cannot open directory list!");

    /* Loop over directories... */
    while (fscanf(in, "%s", wrkdir) != EOF) {

      /* Write info... */
      LOG(1, "\nWorking directory: %s", wrkdir);

      /* Call forward model... */
      call_formod(&ctl, wrkdir, argv[2], argv[3], argv[4], task);
    }

    /* Close dirlist... */
    fclose(in);
  }

#endif

  return EXIT_SUCCESS;
}

/*****************************************************************************/

void call_formod(
  ctl_t * ctl,
  const char *wrkdir,
  const char *obsfile,
  const char *atmfile,
  const char *radfile,
  const char *task) {

  static atm_t atm, atm2;
  static obs_t obs, obs2;
```

```

  char filename[LEN];

  /* Read observation geometry... */
  read_obs(wrkdir, obsfile, ctl, &obs);

  /* Read atmospheric data... */
  read_atm(wrkdir, atmfile, ctl, &atm);

  /* Compute multiple profiles... */
  if (task[0] == 'p' || task[0] == 'P') {

    /* Loop over ray paths... */
    for (int ir = 0; ir < obs.nr; ir++) {

      /* Get atmospheric data... */
      atm2.np = 0;
      for (int ip = 0; ip < atm.np; ip++)
        if (atm.time[ip] == obs.time[ir]) {
          atm2.time[atm2.np] = atm.time[ip];
          atm2.z[atm2.np] = atm.z[ip];
          atm2.lon[atm2.np] = atm.lon[ip];
          atm2.lat[atm2.np] = atm.lat[ip];
          atm2.p[atm2.np] = atm.p[ip];
          atm2.t[atm2.np] = atm.t[ip];
          for (int ig = 0; ig < ctl->ng; ig++)
            atm2.q[ig][atm2.np] = atm.q[ig][ip];
          for (int iw = 0; iw < ctl->nw; iw++)
            atm2.k[iw][atm2.np] = atm.k[iw][ip];
          atm2.np++;
        }

      /* Get observation data... */
      obs2.nr = 1;
      obs2.time[0] = obs.time[ir];
      obs2.vpz[0] = obs.vpz[ir];
      obs2.vplon[0] = obs.vplon[ir];
      obs2.vplat[0] = obs.vplat[ir];
      obs2.obsz[0] = obs.obsz[ir];
      obs2.obslon[0] = obs.obslon[ir];
      obs2.obslat[0] = obs.obslat[ir];

      /* Check number of data points... */
      if (atm2.np > 0) {

        /* Call forward model... */
        formod(ctl, &atm2, &obs2);

        /* Save radiance data... */
        for (int id = 0; id < ctl->nd; id++) {
          obs.rad[id][ir] = obs2.rad[id][0];
          obs.tau[id][ir] = obs2.tau[id][0];
        }
      }
    }

    /* Write radiance data... */
    write_obs(wrkdir, radfile, ctl, &obs);
  }

  /* Compute single profile... */
  else {

    /* Call forward model... */
    formod(ctl, &atm, &obs);

    /* Save radiance data... */
    write_obs(wrkdir, radfile, ctl, &obs);

    /* Compute contributions... */
    if (task[0] == 'c' || task[0] == 'C') {

      /* Switch off continua... */
      ctl->ctm_co2 = 0;
      ctl->ctm_h2o = 0;
      ctl->ctm_n2 = 0;
      ctl->ctm_o2 = 0;

      /* Loop over emitters... */
      for (int ig = 0; ig < ctl->ng; ig++) {

        /* Copy atmospheric data... */
        copy_atm(ctl, &atm2, &atm, 0);

        /* Set extinction to zero... */
        for (int iw = 0; iw < ctl->nw; iw++)
          for (int ip = 0; ip < atm2.np; ip++)
```

```
          atm2.k[iw][ip] = 0;

        /* Set volume mixing ratios to zero... */
        for (int ig2 = 0; ig2 < ctl->ng; ig2++)
          if (ig2 != ig)
            for (int ip = 0; ip < atm2.np; ip++)
              atm2.q[ig2][ip] = 0;

        /* Call forward model... */
        formod(ctl, &atm2, &obs);

        /* Save radiance data... */
        sprintf(filename, "%s.%s", radfile, ctl->emitter[ig]);
        write_obs(wrkdir, filename, ctl, &obs);
      }

      /* Copy atmospheric data... */
      copy_atm(ctl, &atm2, &atm, 0);

      /* Set volume mixing ratios to zero... */
      for (int ig = 0; ig < ctl->ng; ig++)
        for (int ip = 0; ip < atm2.np; ip++)
          atm2.q[ig][ip] = 0;

      /* Call forward model... */
      formod(ctl, &atm2, &obs);

      /* Save radiance data... */
      sprintf(filename, "%s.EXTINCT", radfile);
      write_obs(wrkdir, filename, ctl, &obs);
    }

    /* Measure CPU-time... */
    if (task[0] == 't' || task[0] == 'T') {

      /* Init... */
      double t_min, t_max, t_mean = 0, t_sigma = 0;
      int n = 0;

      /* Initialize random number generator... */
      gsl_rng_env_setup();
      gsl_rng *rng = gsl_rng_alloc(gsl_rng_default);

      /* Loop over profiles... */
      do {

        /* Create random atmosphere... */
        copy_atm(ctl, &atm2, &atm, 0);
        double dtemp = 40. * (gsl_rng_uniform(rng) - 0.5);
        double dpress = 1. - 0.1 * gsl_rng_uniform(rng);
        double dq[NG];
        for (int ig = 0; ig < ctl->ng; ig++)
          dq[ig] = 0.8 + 0.4 * gsl_rng_uniform(rng);
        for (int ip = 0; ip < atm2.np; ip++) {
          atm.t[ip] += dtemp;
          atm.p[ip] *= dpress;
          for (int ig = 0; ig < ctl->ng; ig++)
            atm.q[ig][ip] *= dq[ig];
        }

        /* Measure runtime... */
        double t0 = omp_get_wtime();
        formod(ctl, &atm2, &obs);
        double dt = omp_get_wtime() - t0;

        /* Get runtime statistics... */
        t_mean += (dt);
        t_sigma += POW2(dt);
        if (n == 0 || dt < t_min)
          t_min = dt;
        if (n == 0 || dt > t_max)
          t_max = dt;
        n++;

      } while (t_mean < 10.0);

      /* Write results... */
      t_mean /= (double) n;
      t_sigma = sqrt(t_sigma / (double) n - POW2(t_mean));
      printf("RUNTIME_MEAN = %g s\n", t_mean);
      printf("RUNTIME_SIGMA = %g s\n", t_sigma);
      printf("RUNTIME_MIN = %g s\n", t_min);
      printf("RUNTIME_MAX = %g s\n", t_max);
      printf("RAYS_PER_SECOND = %g", (double) obs.nr / t_mean);
    }

    /* Analyze effect of step size... */
```

```
    if (task[0] == 's' || task[0] == 'S') {

      /* Reference run... */
      ctl->rayds = 0.1;
      ctl->raydz = 0.01;
      formod(ctl, &atm, &obs);
      copy_obs(ctl, &obs2, &obs, 0);

      /* Loop over step size... */
      for (double dz = 0.01; dz <= 2; dz *= 1.1) {
        printf("STEPSIZE: \n");
        for (double ds = 0.1; ds <= 50; ds *= 1.1) {

          /* Set step size... */
          ctl->rayds = ds;
          ctl->raydz = dz;

          /* Measure runtime... */
          double t0 = omp_get_wtime();
          formod(ctl, &atm, &obs);
          double dt = omp_get_wtime() - t0;

          /* Get differences... */
          double mean[ND], sigma[ND];
          for (int id = 0; id < ctl->nd; id++) {
            mean[id] = sigma[id] = 0;
            int n = 0;
            for (int ir = 0; ir < obs.nr; ir++) {
              double err = 200. * (obs.rad[id][ir] - obs2.rad[id][ir])
                / (obs.rad[id][ir] + obs2.rad[id][ir]);
              mean[id] += err;
              sigma[id] += POW2(err);
              n++;
            }
            mean[id] /= n;
            sigma[id] = sqrt(sigma[id] / n - POW2(mean[id]));
          }

          /* Write results... */
          printf("STEPSIZE: %g %g %g", ds, dz, dt);
          for (int id = 0; id < ctl->nd; id++)
            printf(" %g %g", mean[id], sigma[id]);
          printf("\n");
        }
      }
    }
  }
}
```

5.9 hydrostatic.c File Reference

Recalculate pressure based on hydrostatic equilibrium.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.9.1 Detailed Description

Recalculate pressure based on hydrostatic equilibrium.

Definition in file hydrostatic.c.

5.9.2 Function Documentation

5.9.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file hydrostatic.c.

```
                  {

  static atm_t atm;
  static ctl_t ctl;

  /* Check arguments... */
  if (argc < 4)
    ERRMSG("Give parameters: <ctl> <atm_in> <atm_hyd>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Check reference height... */
  if (ctl.hydz < 0)
    ERRMSG("Set HYDZ>=0!");

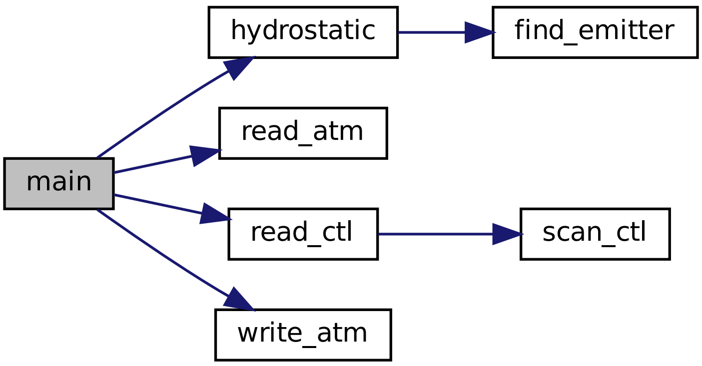
  /* Read atmospheric data... */
  read_atm(NULL, argv[2], &ctl, &atm);

  /* Build atmosphere based on hydrostatic equilibrium... */
  hydrostatic(&ctl, &atm);

  /* Write atmospheric data... */
  write_atm(NULL, argv[3], &ctl, &atm);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.10 hydrostatic.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
```

```
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static atm_t atm;
  static ctl_t ctl;

  /* Check arguments... */
  if (argc < 4)
    ERRMSG("Give parameters: <ctl> <atm_in> <atm_hyd>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Check reference height... */
  if (ctl.hydz < 0)
    ERRMSG("Set HYDZ>=0!");

  /* Read atmospheric data... */
  read_atm(NULL, argv[2], &ctl, &atm);

  /* Build atmosphere based on hydrostatic equilibrium... */
  hydrostatic(&ctl, &atm);

  /* Write atmospheric data... */
  write_atm(NULL, argv[3], &ctl, &atm);

  return EXIT_SUCCESS;
}
```

5.11 interpolate.c File Reference

Interpolate atmospheric data to another spatial grid.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.11.1 Detailed Description

Interpolate atmospheric data to another spatial grid.

Definition in file interpolate.c.

5.11.2 Function Documentation

5.11.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file interpolate.c.

```
                      {

  static atm_t atm_in, atm_pts;
  static ctl_t ctl;

  double k[NW], q[NG];

  /* Interpolate atmospheric data... */

  /* Check arguments... */
  if (argc < 5)
    ERRMSG("Give parameters: <ctl> <atm_in> <atm_pts> <atm_out>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

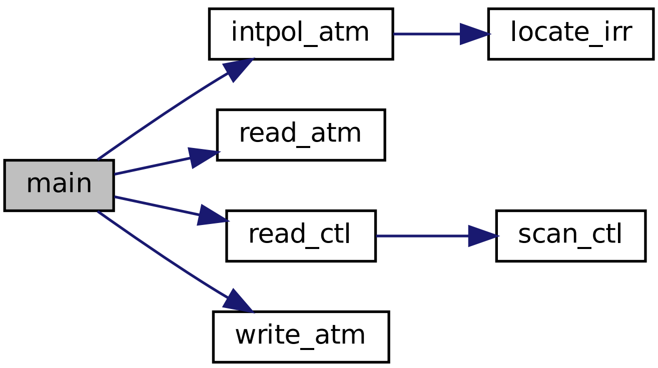
  /* Read atmospheric data... */
  read_atm(NULL, argv[2], &ctl, &atm_in);
  read_atm(NULL, argv[3], &ctl, &atm_pts);

  /* Interpolate atmospheric data... */
  for (int ip = 0; ip < atm_pts.np; ip++) {
    intpol_atm(&ctl, &atm_in, atm_pts.z[ip],
               &atm_pts.p[ip], &atm_pts.t[ip], q, k);
    for (int ig = 0; ig < ctl.ng; ig++)
      atm_pts.q[ig][ip] = q[ig];
    for (int iw = 0; iw < ctl.nw; iw++)
      atm_pts.k[iw][ip] = k[iw];
  }

  /* Save interpolated data... */
  write_atm(NULL, argv[4], &ctl, &atm_pts);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.12 interpolate.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
```

```
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static atm_t atm_in, atm_pts;
  static ctl_t ctl;

  double k[NW], q[NG];

  /* Interpolate atmospheric data... */

  /* Check arguments... */
  if (argc < 5)
    ERRMSG("Give parameters: <ctl> <atm_in> <atm_pts> <atm_out>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Read atmospheric data... */
  read_atm(NULL, argv[2], &ctl, &atm_in);
  read_atm(NULL, argv[3], &ctl, &atm_pts);

  /* Interpolate atmospheric data... */
  for (int ip = 0; ip < atm_pts.np; ip++) {
    intpol_atm(&ctl, &atm_in, atm_pts.z[ip],
               &atm_pts.p[ip], &atm_pts.t[ip], q, k);
    for (int ig = 0; ig < ctl.ng; ig++)
      atm_pts.q[ig][ip] = q[ig];
    for (int iw = 0; iw < ctl.nw; iw++)
      atm_pts.k[iw][ip] = k[iw];
  }

  /* Save interpolated data... */
  write_atm(NULL, argv[4], &ctl, &atm_pts);

  return EXIT_SUCCESS;
}
```

5.13 invert.c File Reference

Inversion tool for MPTRAC.

```
#include "jurassic.h"
#include <gsl/gsl_fit.h>
```

Macros

- #define NLMAX 30000000

  Maximum number of data lines...
- #define NMAX 1000

  Maximum number of data points...

Functions

- int main (int argc, char *argv[ ])

5.13.1 Detailed Description

Inversion tool for MPTRAC.

Definition in file invert.c.

5.13.2 Macro Definition Documentation

5.13.2.1 NLMAX `#define NLMAX 30000000`

Maximum number of data lines...

Definition at line 33 of file invert.c.

5.13.2.2 NMAX `#define NMAX 1000`

Maximum number of data points...

Definition at line 36 of file invert.c.

5.13.3 Function Documentation

5.13.3.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 42 of file invert.c.

```
                  {

  static ctl_t ctl;

  static atm_t atm, atm2;

  static obs_t obs;

  static gsl_matrix *k;

  static FILE *in, *out;

  static char line[LEN];

  static double rtime[NLMAX], rz[NLMAX], rlon[NLMAX], rlat[NLMAX], obs_meas,
    obs_sim, scl = 1.0, scl_old, scl_err, c0, c1, cov00, cov01, cov11,
    sumsq, x[NMAX], x2[NMAX], y[NMAX], y_err[NMAX], y2[NMAX], y2_err[NMAX],
    y2_sim[NMAX], y2_sim_err[NMAX], w2[NMAX], dt, tol, obs_err;

  static float rp[NLMAX], rt[NLMAX], rso2[NLMAX], rh2o[NLMAX],
    ro3[NLMAX], robs[NLMAX];

  static int data, fit, i, ig, il, ip, it, itmax, n, nl, ndata[NMAX], nprof;

  static size_t mk, nk;

  /* Check arguments... */
```

```
  if (argc < 6)
    ERRMSG("Give parameters: <ctl> <prof> <inv> <atm> <kernel>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  dt = scan_ctl(argc, argv, "INVERT_DT", -1, "86400", NULL);
  obs_err = scan_ctl(argc, argv, "INVERT_OBS_ERR", -1, "1.0", NULL);
  data = (int) scan_ctl(argc, argv, "INVERT_DATA", -1, "2", NULL);
  fit = (int) scan_ctl(argc, argv, "INVERT_FIT", -1, "3", NULL);
  itmax = (int) scan_ctl(argc, argv, "INVERT_ITMAX", -1, "10", NULL);
  tol = scan_ctl(argc, argv, "INVERT_TOL", -1, "1e-4", NULL);

  /* Check control parameters... */
  if (ctl.ng != 4)
    ERRMSG("Set NG = 4!");
  if (strcmp(ctl.emitter[0], "SO2") != 0)
    ERRMSG("Set EMITTER[0] = SO2!");
  if (strcmp(ctl.emitter[1], "H2O") != 0)
    ERRMSG("Set EMITTER[1] = H2O!");
  if (strcmp(ctl.emitter[2], "O3") != 0)
    ERRMSG("Set EMITTER[2] = O3!");
  if (strcmp(ctl.emitter[3], "CO2") != 0)
    ERRMSG("Set EMITTER[3] = CO2!");
  if (ctl.nd != 2)
    ERRMSG("Set ND = 2!");

  /* Set control parameters... */
  ctl.write_bbt = 1;
  ctl.write_matrix = 1;

  /* Set observation data... */
  obs.nr = 1;
  obs.obsz[0] = 705;

  /* ------------------------------------------------------------
     Read profiles...
     ------------------------------------------------------------ */

  /* Read profile data... */
  LOG(1, "Read profile data: %s", argv[2]);

  /* Open file... */
  if (!(in = fopen(argv[2], "r")))
    ERRMSG("Cannot open file!");

  /* Read file... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    if (sscanf(line, "%lg %lg %lg %lg %g %g %g %g %g %g", &rtime[nl],
               &rz[nl], &rlon[nl], &rlat[nl], &rp[nl], &rt[nl], &rso2[nl],
               &rh2o[nl], &ro3[nl], &robs[nl]) != 10)
      continue;
    if ((++nl) > NLMAX)
      ERRMSG("Too many profile data points!");
  }

  /* Close files... */
  fclose(in);

  /* ------------------------------------------------------------
     Fit scaling factor for total mass...
     ------------------------------------------------------------ */

  /* Iterations... */
  for (it = 0; it < itmax; it++) {

    /* Init... */
    atm.np = n = 0;
    for (i = 0; i < NMAX; i++) {
      ndata[i] = 0;
      x[i] = y[i] = GSL_NAN;
    }

    /* Loop over lines... */
    for (il = 0; il < nl; il++) {

      /* Check for new profile... */
      if ((rtime[il] != atm.time[0]
           || rlon[il] != atm.lon[0]
           || rlat[il] != atm.lat[0])
          && atm.np > 0) {

        /* Call forward model... */
        formod(&ctl, &atm, &obs);
        obs_sim = obs.rad[0][0] - obs.rad[1][0];

```

```
      /* Get time index... */
      i = (int) ((atm.time[0] - rtime[0]) / dt);
      if (i < 0 && i >= NMAX)
        ERRMSG("Time index out of range!");

      /* Get maxima... */
      if (data == 1) {
        x[i] = (gsl_finite(x[i]) ? GSL_MAX(x[i], obs_sim) : obs_sim);
        y[i] = (gsl_finite(y[i]) ? GSL_MAX(y[i], obs_meas) : obs_meas);
        y_err[i] = obs_err;
        if (gsl_finite(x[i]) && gsl_finite(y[i]))
          ndata[i] = 1;
      }

      /* Get means... */
      else if (data == 2) {
        if (ndata[i] == 0) {
          x[i] = obs_sim;
          y[i] = obs_meas;
          y_err[i] = POW2(obs_meas);
        } else {
          x[i] += obs_sim;
          y[i] += obs_meas;
          y_err[i] += POW2(obs_meas);
        }
        ndata[i]++;
      }

      /* Calculate mean atmospheric profile... */
      nprof++;
      atm2.np = atm.np;
      for (ip = 0; ip < atm.np; ip++) {
        atm2.time[ip] += atm.time[ip];
        atm2.z[ip] += atm.z[ip];
        atm2.lon[ip] += atm.lon[ip];
        atm2.lat[ip] += atm.lat[ip];
        atm2.p[ip] += atm.p[ip];
        atm2.t[ip] += atm.t[ip];
        for (ig = 1; ig < ctl.ng; ig++)
          atm2.q[ig][ip] += atm.q[ig][ip];
      }

      /* Reset counter... */
      atm.np = 0;
    }

    /* Save data... */
    obs_meas = robs[il];
    atm.time[atm.np] = rtime[il];
    atm.z[atm.np] = rz[il];
    atm.lon[atm.np] = rlon[il];
    atm.lat[atm.np] = rlat[il];
    atm.p[atm.np] = rp[il];
    atm.t[atm.np] = rt[il];
    atm.q[0][atm.np] = rso2[il] * scl;
    atm.q[1][atm.np] = rh2o[il];
    atm.q[2][atm.np] = ro3[il];
    atm.q[3][atm.np] = 371.789948e-6 + 2.026214e-6
      * (atm.time[atm.np] - 63158400.) / 31557600.;
    if ((++atm.np) > NP)
      ERRMSG("Too many data points!");
  }

  /* Calculate means... */
  if (data == 2)
    for (i = 0; i < NMAX; i++)
      if (ndata[i] > 0) {
        x[i] /= ndata[i];
        y[i] /= ndata[i];
        y_err[i] = sqrt(GSL_MAX(y_err[i] / ndata[i] - POW2(y[i]), 0.0))
          / sqrt(ndata[i]);    /* standard error! */
      }

  /* Filter data... */
  n = 0;
  for (i = 0; i < NMAX; i++)
    if (ndata[i] > 0 && gsl_finite(x[i]) && gsl_finite(y[i])
        && gsl_finite(y_err[i])) {
      x2[n] = x[i];
      y2[n] = y[i];
      y2_err[n] = y_err[i];
      w2[n] = 1. / POW2(y_err[i]);
      n++;
    }

  /* Fit radiance data... */
  if (fit == 1)
```

```
      gsl_fit_mul(x2, 1, y2, 1, (size_t) n, &c1, &cov11, &sumsq);
    else if (fit == 2)
      gsl_fit_wmul(x2, 1, w2, 1, y2, 1, (size_t) n, &c1, &cov11, &sumsq);
    else if (fit == 3)
      gsl_fit_linear(x2, 1, y2, 1, (size_t) n, &c0, &c1, &cov00, &cov01,
                     &cov11, &sumsq);
    else if (fit == 4)
      gsl_fit_wlinear(x2, 1, w2, 1, y2, 1, (size_t) n, &c0, &c1, &cov00,
                      &cov01, &cov11, &sumsq);
    else
      ERRMSG("Check INVERT_FIT!");

    /* Get new scaling factor... */
    scl_old = scl;
    scl_err = scl * sqrt(cov11);
    scl *= c1;

    /* Write info... */
    LOG(1, "  it= %d | scl= %g +/- %g | RMSE= %g",
        it, scl, scl_err, sqrt(sumsq / n));

    /* Convergence test... */
    if (fabs(2.0 * (scl - scl_old) / (scl + scl_old)) < tol)
      break;
  }

  /* ------------------------------------------------------------
     Write inversion data...
     ------------------------------------------------------------ */

  /* Write info... */
  LOG(1, "Write inversion data: %s", argv[3]);

  /* Create file... */
  if (!(out = fopen(argv[3], "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = simulated SO2 index [K]\n"
          "# $3 = scaled simulated SO2 index [K]\n"
          "# $4 = error of scaled simulated SO2 index [K]\n"
          "# $5 = observed SO2 index [K]\n"
          "# $6 = error of observed SO2 index [K]\n\n");

  /* Write data... */
  for (i = 0; i < n; i++) {

    /* Calculate scaled SO2 index... */
    if (fit == 1 || fit == 2)
      gsl_fit_mul_est(x2[i], c1, cov11, &y2_sim[i], &y2_sim_err[i]);
    else if (fit == 3 || fit == 4)
      gsl_fit_linear_est(x2[i], c0, c1, cov00, cov01, cov11, &y2_sim[i],
                         &y2_sim_err[i]);

    /* Write output... */
    fprintf(out, "%.2f %g %g %g %g %g\n", rtime[0] + (i + 0.5) * dt,
            x2[i], y2_sim[i], y2_sim_err[i], y2[i], y2_err[i]);
  }

  /* Report scaling factor for total mass... */
  fprintf(out, "\n");
  fprintf(out, "#    scl= %g +/- %g\n", scl, scl_err);
  fprintf(out, "#     c1= %g +/- %g\n", c1, sqrt(cov11));
  if (fit == 3 || fit == 4) {
    fprintf(out, "#     c0= %g +/- %g\n", c0, sqrt(cov00));
    fprintf(out, "#   corr= %g\n", cov01 / (sqrt(cov00) * sqrt(cov11)));
  }
  fprintf(out, "#   RMSE= %g\n", sqrt(sumsq / n));
  fprintf(out, "#      n= %d\n", n);

  /* Close files... */
  fclose(out);

  /* ------------------------------------------------------------
     Calculate kernel...
     ------------------------------------------------------------ */

  /* Set atmospheric data... */
  for (ip = 0; ip < atm2.np; ip++) {
    atm2.time[ip] /= nprof;
    atm2.z[ip] /= nprof;
    atm2.lon[ip] /= nprof;
    atm2.lat[ip] /= nprof;
    atm2.p[ip] /= nprof;
    atm2.t[ip] /= nprof;
```

```
    for (ig = 0; ig < ctl.ng; ig++)
      atm2.q[ig][ip] /= nprof;
  }

  /* Get sizes... */
  nk = atm2x(&ctl, &atm2, NULL, NULL, NULL);
  mk = obs2y(&ctl, &obs, NULL, NULL, NULL);

  /* Allocate... */
  k = gsl_matrix_alloc(mk, nk);

  /* Compute kernel matrix... */
  kernel(&ctl, &atm2, &obs, k);

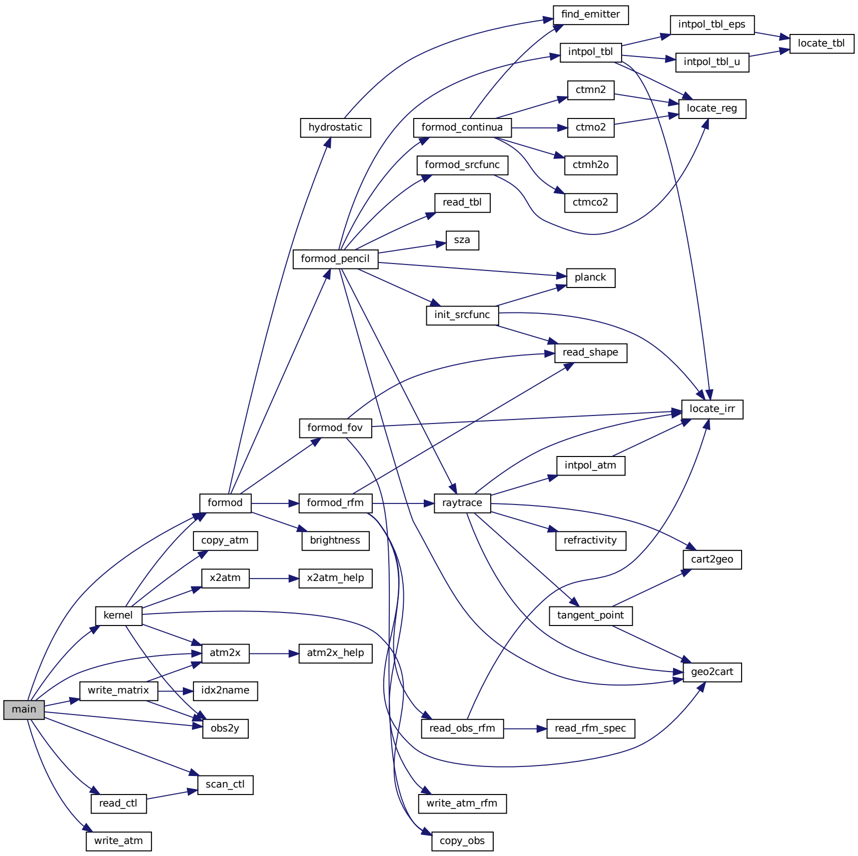
  /* Write atmospheric data... */
  write_atm(NULL, argv[4], &ctl, &atm);

  /* Write matrix to file... */
  write_matrix(NULL, argv[5], &ctl, k, &atm2, &obs, "y", "x", "r");

  /* Free... */
  gsl_matrix_free(k);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.14 invert.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.
```

```
  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2019-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"
#include <gsl/gsl_fit.h>

/* ------------------------------------------------------------
   Constants...
   ------------------------------------------------------------ */

#define NLMAX 30000000

#define NMAX 1000

/* ------------------------------------------------------------
   Main...
   ------------------------------------------------------------ */

int main(
  int argc,
  char *argv[]) {

  static ctl_t ctl;

  static atm_t atm, atm2;

  static obs_t obs;

  static gsl_matrix *k;

  static FILE *in, *out;

  static char line[LEN];

  static double rtime[NLMAX], rz[NLMAX], rlon[NLMAX], rlat[NLMAX], obs_meas,
    obs_sim, scl = 1.0, scl_old, scl_err, c0, c1, cov00, cov01, cov11,
    sumsq, x[NMAX], x2[NMAX], y[NMAX], y_err[NMAX], y2[NMAX], y2_err[NMAX],
    y2_sim[NMAX], y2_sim_err[NMAX], w2[NMAX], dt, tol, obs_err;

  static float rp[NLMAX], rt[NLMAX], rso2[NLMAX], rh2o[NLMAX],
    ro3[NLMAX], robs[NLMAX];

  static int data, fit, i, ig, il, ip, it, itmax, n, nl, ndata[NMAX], nprof;

  static size_t mk, nk;

  /* Check arguments... */
  if (argc < 6)
    ERRMSG("Give parameters: <ctl> <prof> <inv> <atm> <kernel>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  dt = scan_ctl(argc, argv, "INVERT_DT", -1, "86400", NULL);
  obs_err = scan_ctl(argc, argv, "INVERT_OBS_ERR", -1, "1.0", NULL);
  data = (int) scan_ctl(argc, argv, "INVERT_DATA", -1, "2", NULL);
  fit = (int) scan_ctl(argc, argv, "INVERT_FIT", -1, "3", NULL);
  itmax = (int) scan_ctl(argc, argv, "INVERT_ITMAX", -1, "10", NULL);
  tol = scan_ctl(argc, argv, "INVERT_TOL", -1, "1e-4", NULL);

  /* Check control parameters... */
  if (ctl.ng != 4)
    ERRMSG("Set NG = 4!");
  if (strcmp(ctl.emitter[0], "SO2") != 0)
    ERRMSG("Set EMITTER[0] = SO2!");
  if (strcmp(ctl.emitter[1], "H2O") != 0)
    ERRMSG("Set EMITTER[1] = H2O!");
  if (strcmp(ctl.emitter[2], "O3") != 0)
    ERRMSG("Set EMITTER[2] = O3!");
  if (strcmp(ctl.emitter[3], "CO2") != 0)
    ERRMSG("Set EMITTER[3] = CO2!");
  if (ctl.nd != 2)
    ERRMSG("Set ND = 2!");

  /* Set control parameters... */
  ctl.write_bbt = 1;
  ctl.write_matrix = 1;

  /* Set observation data... */
```

```
  obs.nr = 1;
  obs.obsz[0] = 705;

  /* ------------------------------------------------------------
     Read profiles...
     ------------------------------------------------------------ */

  /* Read profile data... */
  LOG(1, "Read profile data: %s", argv[2]);

  /* Open file... */
  if (!(in = fopen(argv[2], "r")))
    ERRMSG("Cannot open file!");

  /* Read file... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    if (sscanf(line, "%lg %lg %lg %lg %g %g %g %g %g %g", &rtime[nl],
               &rz[nl], &rlon[nl], &rlat[nl], &rp[nl], &rt[nl], &rso2[nl],
               &rh2o[nl], &ro3[nl], &robs[nl]) != 10)
      continue;
    if ((++nl) > NLMAX)
      ERRMSG("Too many profile data points!");
  }

  /* Close files... */
  fclose(in);

  /* ------------------------------------------------------------
     Fit scaling factor for total mass...
     ------------------------------------------------------------ */

  /* Iterations... */
  for (it = 0; it < itmax; it++) {

    /* Init... */
    atm.np = n = 0;
    for (i = 0; i < NMAX; i++) {
      ndata[i] = 0;
      x[i] = y[i] = GSL_NAN;
    }

    /* Loop over lines... */
    for (il = 0; il < nl; il++) {

      /* Check for new profile... */
      if ((rtime[il] != atm.time[0]
           || rlon[il] != atm.lon[0]
           || rlat[il] != atm.lat[0])
          && atm.np > 0) {

        /* Call forward model... */
        formod(&ctl, &atm, &obs);
        obs_sim = obs.rad[0][0] - obs.rad[1][0];

        /* Get time index... */
        i = (int) ((atm.time[0] - rtime[0]) / dt);
        if (i < 0 && i >= NMAX)
          ERRMSG("Time index out of range!");

        /* Get maxima... */
        if (data == 1) {
          x[i] = (gsl_finite(x[i]) ? GSL_MAX(x[i], obs_sim) : obs_sim);
          y[i] = (gsl_finite(y[i]) ? GSL_MAX(y[i], obs_meas) : obs_meas);
          y_err[i] = obs_err;
          if (gsl_finite(x[i]) && gsl_finite(y[i]))
            ndata[i] = 1;
        }

        /* Get means... */
        else if (data == 2) {
          if (ndata[i] == 0) {
            x[i] = obs_sim;
            y[i] = obs_meas;
            y_err[i] = POW2(obs_meas);
          } else {
            x[i] += obs_sim;
            y[i] += obs_meas;
            y_err[i] += POW2(obs_meas);
          }
          ndata[i]++;
        }

        /* Calculate mean atmospheric profile... */
        nprof++;
        atm2.np = atm.np;
```

```
        for (ip = 0; ip < atm.np; ip++) {
          atm2.time[ip] += atm.time[ip];
          atm2.z[ip] += atm.z[ip];
          atm2.lon[ip] += atm.lon[ip];
          atm2.lat[ip] += atm.lat[ip];
          atm2.p[ip] += atm.p[ip];
          atm2.t[ip] += atm.t[ip];
          for (ig = 1; ig < ctl.ng; ig++)
            atm2.q[ig][ip] += atm.q[ig][ip];
        }

        /* Reset counter... */
        atm.np = 0;
      }

      /* Save data... */
      obs_meas = robs[il];
      atm.time[atm.np] = rtime[il];
      atm.z[atm.np] = rz[il];
      atm.lon[atm.np] = rlon[il];
      atm.lat[atm.np] = rlat[il];
      atm.p[atm.np] = rp[il];
      atm.t[atm.np] = rt[il];
      atm.q[0][atm.np] = rso2[il] * scl;
      atm.q[1][atm.np] = rh2o[il];
      atm.q[2][atm.np] = ro3[il];
      atm.q[3][atm.np] = 371.789948e-6 + 2.026214e-6
        * (atm.time[atm.np] - 63158400.) / 31557600.;
      if ((++atm.np) > NP)
        ERRMSG("Too many data points!");
    }

    /* Calculate means... */
    if (data == 2)
      for (i = 0; i < NMAX; i++)
        if (ndata[i] > 0) {
          x[i] /= ndata[i];
          y[i] /= ndata[i];
          y_err[i] = sqrt(GSL_MAX(y_err[i] / ndata[i] - POW2(y[i]), 0.0))
            / sqrt(ndata[i]);   /* standard error! */
        }

    /* Filter data... */
    n = 0;
    for (i = 0; i < NMAX; i++)
      if (ndata[i] > 0 && gsl_finite(x[i]) && gsl_finite(y[i])
          && gsl_finite(y_err[i])) {
        x2[n] = x[i];
        y2[n] = y[i];
        y2_err[n] = y_err[i];
        w2[n] = 1. / POW2(y_err[i]);
        n++;
      }

    /* Fit radiance data... */
    if (fit == 1)
      gsl_fit_mul(x2, 1, y2, 1, (size_t) n, &c1, &cov11, &sumsq);
    else if (fit == 2)
      gsl_fit_wmul(x2, 1, w2, 1, y2, 1, (size_t) n, &c1, &cov11, &sumsq);
    else if (fit == 3)
      gsl_fit_linear(x2, 1, y2, 1, (size_t) n, &c0, &c1, &cov00, &cov01,
                     &cov11, &sumsq);
    else if (fit == 4)
      gsl_fit_wlinear(x2, 1, w2, 1, y2, 1, (size_t) n, &c0, &c1, &cov00,
                      &cov01, &cov11, &sumsq);
    else
      ERRMSG("Check INVERT_FIT!");

    /* Get new scaling factor... */
    scl_old = scl;
    scl_err = scl * sqrt(cov11);
    scl *= c1;

    /* Write info... */
    LOG(1, "  it= %d | scl= %g +/- %g | RMSE= %g",
        it, scl, scl_err, sqrt(sumsq / n));

    /* Convergence test... */
    if (fabs(2.0 * (scl - scl_old) / (scl + scl_old)) < tol)
      break;
  }

  /* ------------------------------------------------------------
     Write inversion data...
     ------------------------------------------------------------ */

  /* Write info... */
```

```
  LOG(1, "Write inversion data: %s", argv[3]);

  /* Create file... */
  if (!(out = fopen(argv[3], "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = simulated SO2 index [K]\n"
          "# $3 = scaled simulated SO2 index [K]\n"
          "# $4 = error of scaled simulated SO2 index [K]\n"
          "# $5 = observed SO2 index [K]\n"
          "# $6 = error of observed SO2 index [K]\n\n");

  /* Write data... */
  for (i = 0; i < n; i++) {

    /* Calculate scaled SO2 index... */
    if (fit == 1 || fit == 2)
      gsl_fit_mul_est(x2[i], c1, cov11, &y2_sim[i], &y2_sim_err[i]);
    else if (fit == 3 || fit == 4)
      gsl_fit_linear_est(x2[i], c0, c1, cov00, cov01, cov11, &y2_sim[i],
                         &y2_sim_err[i]);

    /* Write output... */
    fprintf(out, "%.2f %g %g %g %g %g\n", rtime[0] + (i + 0.5) * dt,
            x2[i], y2_sim[i], y2_sim_err[i], y2[i], y2_err[i]);
  }

  /* Report scaling factor for total mass... */
  fprintf(out, "\n");
  fprintf(out, "#    scl= %g +/- %g\n", scl, scl_err);
  fprintf(out, "#     c1= %g +/- %g\n", c1, sqrt(cov11));
  if (fit == 3 || fit == 4) {
    fprintf(out, "#     c0= %g +/- %g\n", c0, sqrt(cov00));
    fprintf(out, "#   corr= %g\n", cov01 / (sqrt(cov00) * sqrt(cov11)));
  }
  fprintf(out, "#   RMSE= %g\n", sqrt(sumsq / n));
  fprintf(out, "#      n= %d\n", n);

  /* Close files... */
  fclose(out);

  /* ------------------------------------------------------------
     Calculate kernel...
     ------------------------------------------------------------ */

  /* Set atmospheric data... */
  for (ip = 0; ip < atm2.np; ip++) {
    atm2.time[ip] /= nprof;
    atm2.z[ip] /= nprof;
    atm2.lon[ip] /= nprof;
    atm2.lat[ip] /= nprof;
    atm2.p[ip] /= nprof;
    atm2.t[ip] /= nprof;
    for (ig = 0; ig < ctl.ng; ig++)
      atm2.q[ig][ip] /= nprof;
  }

  /* Get sizes... */
  nk = atm2x(&ctl, &atm2, NULL, NULL, NULL);
  mk = obs2y(&ctl, &obs, NULL, NULL, NULL);

  /* Allocate... */
  k = gsl_matrix_alloc(mk, nk);

  /* Compute kernel matrix... */
  kernel(&ctl, &atm2, &obs, k);

  /* Write atmospheric data... */
  write_atm(NULL, argv[4], &ctl, &atm);

  /* Write matrix to file... */
  write_matrix(NULL, argv[5], &ctl, k, &atm2, &obs, "y", "x", "r");

  /* Free... */
  gsl_matrix_free(k);

  return EXIT_SUCCESS;
}
```

5.15 jsec2time.c File Reference

Convert Julian seconds to date.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char ∗argv[ ])

5.15.1 Detailed Description

Convert Julian seconds to date.

Definition in file jsec2time.c.

5.15.2 Function Documentation

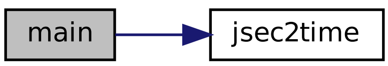
5.15.2.1 main()

```
int main (
    int argc,
    char ∗ argv[ ] )
```

Definition at line 27 of file jsec2time.c.

```
00029                     {
00030
00031   double remain;
00032
00033   int day, hour, min, mon, sec, year;
00034
00035   /* Check arguments... */
00036   if (argc < 2)
00037     ERRMSG("Give parameters: <jsec>");
00038
00039   /* Read arguments... */
00040   double jsec = atof(argv[1]);
00041
00042   /* Convert time... */
00043   jsec2time(jsec, &year, &mon, &day, &hour, &min, &sec, &remain);
00044   printf("%d %d %d %d %d %d %g\n", year, mon, day, hour, min, sec, remain);
00045
00046   return EXIT_SUCCESS;
00047 }
```

Here is the call graph for this function:



5.16 jsec2time.c

```
/*
  This file is part of JURASSIC.

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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

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  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  double remain;

  int day, hour, min, mon, sec, year;

  /* Check arguments... */
  if (argc < 2)
    ERRMSG("Give parameters: <jsec>");

  /* Read arguments... */
  double jsec = atof(argv[1]);

  /* Convert time... */
  jsec2time(jsec, &year, &mon, &day, &hour, &min, &sec, &remain);
  printf("%d %d %d %d %d %d %g\n", year, mon, day, hour, min, sec, remain);

  return EXIT_SUCCESS;
}
```

5.17 jurassic.c File Reference

JURASSIC library definitions.

```
#include "jurassic.h"
```

Functions

- size_t atm2x (ctl_t *ctl, atm_t *atm, gsl_vector *x, int *iqa, int *ipa)

  Compose state vector or parameter vector.
- void atm2x_help (double value, int value_iqa, int value_ip, gsl_vector *x, int *iqa, int *ipa, size_t *n)

  Add element to state vector.
- double brightness (double rad, double nu)

  Compute brightness temperature.
- void cart2geo (double *x, double *z, double *lon, double *lat)

  Convert Cartesian coordinates to geolocation.
- void climatology (ctl_t *ctl, atm_t *atm)

  Interpolate climatological data.
- double ctmco2 (double nu, double p, double t, double u)

  Compute carbon dioxide continuum (optical depth).
- double ctmh2o (double nu, double p, double t, double q, double u)

  Compute water vapor continuum (optical depth).

- double ctmn2 (double nu, double p, double t)

    Compute nitrogen continuum (absorption coefficient).
- double ctmo2 (double nu, double p, double t)

    Compute oxygen continuum (absorption coefficient).
- void copy_atm (ctl_t ∗ctl, atm_t ∗atm_dest, atm_t ∗atm_src, int init)

    Copy and initialize atmospheric data.
- void copy_obs (ctl_t ∗ctl, obs_t ∗obs_dest, obs_t ∗obs_src, int init)

    Copy and initialize observation data.
- int find_emitter (ctl_t ∗ctl, const char ∗emitter)

    Find index of an emitter.
- void formod (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs)

    Determine ray paths and compute radiative transfer.
- void formod_continua (ctl_t ∗ctl, los_t ∗los, int ip, double ∗beta)

    Compute absorption coefficient of continua.
- void formod_fov (ctl_t ∗ctl, obs_t ∗obs)

    Apply field of view convolution.
- void formod_pencil (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs, int ir)

    Compute radiative transfer for a pencil beam.
- void formod_rfm (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs)

    Apply RFM for radiative transfer calculations.
- void formod_srcfunc (ctl_t ∗ctl, tbl_t ∗tbl, double t, double ∗src)

    Compute Planck source function.
- void geo2cart (double z, double lon, double lat, double ∗x)

    Convert geolocation to Cartesian coordinates.
- void hydrostatic (ctl_t ∗ctl, atm_t ∗atm)

    Set hydrostatic equilibrium.
- void idx2name (ctl_t ∗ctl, int idx, char ∗quantity)

    Determine name of state vector quantity for given index.
- void init_srcfunc (ctl_t ∗ctl, tbl_t ∗tbl)

    Initialize source function table.
- void intpol_atm (ctl_t ∗ctl, atm_t ∗atm, double z, double ∗p, double ∗t, double ∗q, double ∗k)

    Interpolate atmospheric data.
- void intpol_tbl (ctl_t ∗ctl, tbl_t ∗tbl, los_t ∗los, int ip, double tau_path[ND][NG], double tau_seg[ND])

    Get transmittance from look-up tables.
- double intpol_tbl_eps (tbl_t ∗tbl, int ig, int id, int ip, int it, double u)

    Interpolate emissivity from look-up tables.
- double intpol_tbl_u (tbl_t ∗tbl, int ig, int id, int ip, int it, double eps)

    Interpolate column density from look-up tables.
- void jsec2time (double jsec, int ∗year, int ∗mon, int ∗day, int ∗hour, int ∗min, int ∗sec, double ∗remain)

    Convert seconds to date.
- void kernel (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs, gsl_matrix ∗k)

    Compute Jacobians.
- int locate_irr (double ∗xx, int n, double x)

    Find array index for irregular grid.
- int locate_reg (double ∗xx, int n, double x)

    Find array index for regular grid.
- int locate_tbl (float ∗xx, int n, double x)

    Find array index in float array.
- size_t obs2y (ctl_t ∗ctl, obs_t ∗obs, gsl_vector ∗y, int ∗ida, int ∗ira)

    Compose measurement vector.
- double planck (double t, double nu)

Compute Planck function.
- void raytrace (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs, los_t ∗los, int ir)

  Do ray-tracing to determine LOS.
- void read_atm (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, atm_t ∗atm)

  Read atmospheric data.
- void read_ctl (int argc, char ∗argv[ ], ctl_t ∗ctl)

  Read forward model control parameters.
- void read_matrix (const char ∗dirname, const char ∗filename, gsl_matrix ∗matrix)

  Read matrix.
- void read_obs (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, obs_t ∗obs)

  Read observation data.
- double read_obs_rfm (const char ∗basename, double z, double ∗nu, double ∗f, int n)

  Read observation data in RFM format.
- void read_rfm_spec (const char ∗filename, double ∗nu, double ∗rad, int ∗npts)

  Read RFM spectrum.
- void read_shape (const char ∗filename, double ∗x, double ∗y, int ∗n)

  Read shape function.
- void read_tbl (ctl_t ∗ctl, tbl_t ∗tbl)

  Read look-up table data.
- double refractivity (double p, double t)

  Compute refractivity (return value is n - 1).
- double scan_ctl (int argc, char ∗argv[ ], const char ∗varname, int arridx, const char ∗defvalue, char ∗value)

  Search control parameter file for variable entry.
- double sza (double sec, double lon, double lat)

  Calculate solar zenith angle.
- void tangent_point (los_t ∗los, double ∗tpz, double ∗tplon, double ∗tplat)

  Find tangent point of a given LOS.
- void time2jsec (int year, int mon, int day, int hour, int min, int sec, double remain, double ∗jsec)

  Convert date to seconds.
- void timer (const char ∗name, const char ∗file, const char ∗func, int line, int mode)

  Measure wall-clock time.
- void write_atm (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, atm_t ∗atm)

  Write atmospheric data.
- void write_atm_rfm (const char ∗filename, ctl_t ∗ctl, atm_t ∗atm)

  Write atmospheric data in RFM format.
- void write_matrix (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, gsl_matrix ∗matrix, atm_t ∗atm, obs_t ∗obs, const char ∗rowspace, const char ∗colspace, const char ∗sort)

  Write matrix.
- void write_obs (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, obs_t ∗obs)

  Write observation data.
- void write_shape (const char ∗filename, double ∗x, double ∗y, int n)

  Write shape function.
- void write_tbl (ctl_t ∗ctl, tbl_t ∗tbl)

  Write look-up table data.
- void x2atm (ctl_t ∗ctl, gsl_vector ∗x, atm_t ∗atm)

  Decompose parameter vector or state vector.
- void x2atm_help (double ∗value, gsl_vector ∗x, size_t ∗n)

  Get element from state vector.
- void y2obs (ctl_t ∗ctl, gsl_vector ∗y, obs_t ∗obs)

  Decompose measurement vector.

5.17.1 Detailed Description

JURASSIC library definitions.

Definition in file jurassic.c.

5.17.2 Function Documentation

5.17.2.1 atm2x()

```
size_t atm2x (
        ctl_t * ctl,
        atm_t * atm,
        gsl_vector * x,
        int * iqa,
        int * ipa )
```

Compose state vector or parameter vector.

Definition at line 29 of file jurassic.c.

```
                {

  size_t n = 0;

  /* Add pressure... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->retp_zmin && atm->z[ip] <= ctl->retp_zmax)
      atm2x_help(atm->p[ip], IDXP, ip, x, iqa, ipa, &n);

  /* Add temperature... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->rett_zmin && atm->z[ip] <= ctl->rett_zmax)
      atm2x_help(atm->t[ip], IDXT, ip, x, iqa, ipa, &n);

  /* Add volume mixing ratios... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retq_zmin[ig]
          && atm->z[ip] <= ctl->retq_zmax[ig])
        atm2x_help(atm->q[ig][ip], IDXQ(ig), ip, x, iqa, ipa, &n);

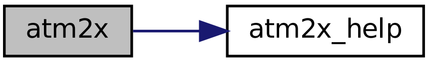
  /* Add extinction... */
  for (int iw = 0; iw < ctl->nw; iw++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retk_zmin[iw]
          && atm->z[ip] <= ctl->retk_zmax[iw])
        atm2x_help(atm->k[iw][ip], IDXK(iw), ip, x, iqa, ipa, &n);

  /* Add cloud parameters... */
  if (ctl->ret_clz)
    atm2x_help(atm->clz, IDXCLZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_cldz)
    atm2x_help(atm->cldz, IDXCLDZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_clk)
    for (int icl = 0; icl < ctl->ncl; icl++)
      atm2x_help(atm->clk[icl], IDXCLK(icl), 0, x, iqa, ipa, &n);

  /* Add surface parameters... */
  if (ctl->ret_sfz)
    atm2x_help(atm->sfz, IDXSFZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_sfp)
    atm2x_help(atm->sfp, IDXSFP, 0, x, iqa, ipa, &n);
  if (ctl->ret_sft)
    atm2x_help(atm->sft, IDXSFT, 0, x, iqa, ipa, &n);
  if (ctl->ret_sfeps)
    for (int isf = 0; isf < ctl->nsf; isf++)
      atm2x_help(atm->sfeps[isf], IDXSFEPS(isf), 0, x, iqa, ipa, &n);

  return n;
}
```

Here is the call graph for this function:



5.17.2.2 atm2x_help()

```
void atm2x_help (
    double value,
    int value_iqa,
    int value_ip,
    gsl_vector * x,
    int * iqa,
    int * ipa,
    size_t * n )
```

Add element to state vector.

Definition at line 87 of file jurassic.c.

```
              {

  /* Add element to state vector... */
  if (x != NULL)
    gsl_vector_set(x, *n, value);
  if (iqa != NULL)
    iqa[*n] = value_iqa;
  if (ipa != NULL)
    ipa[*n] = value_ip;
  (*n)++;
}
```

5.17.2.3 brightness()

```
double brightness (
    double rad,
    double nu )
```

Compute brightness temperature.

Definition at line 109 of file jurassic.c.

```
              {

  return C2 * nu / gsl_log1p(C1 * POW3(nu) / rad);
}
```

5.17.2.4 cart2geo()

```
void cart2geo (
        double * x,
        double * z,
        double * lon,
        double * lat )
```

Convert Cartesian coordinates to geolocation.

Definition at line 119 of file jurassic.c.

```
                  {

  double radius = NORM(x);

  *lat = asin(x[2] / radius) * 180 / M_PI;
  *lon = atan2(x[1], x[0]) * 180 / M_PI;
  *z = radius - RE;
}
```

5.17.2.5 climatology()

```
void climatology (
        ctl_t * ctl,
        atm_t * atm )
```

Interpolate climatological data.

Definition at line 134 of file jurassic.c.

```
                  {

  static double z[121] = {
    0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,
    20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37,
    38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55,
    56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73,
    74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91,
    92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107,
    108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120
  };

  static double pre[121] = {
    1017, 901.083, 796.45, 702.227, 617.614, 541.644, 473.437, 412.288,
    357.603, 308.96, 265.994, 228.348, 195.619, 167.351, 143.039, 122.198,
    104.369, 89.141, 76.1528, 65.0804, 55.641, 47.591, 40.7233, 34.8637,
    29.8633, 25.5956, 21.9534, 18.8445, 16.1909, 13.9258, 11.9913,
    10.34, 8.92988, 7.72454, 6.6924, 5.80701, 5.04654, 4.39238, 3.82902,
    3.34337, 2.92413, 2.56128, 2.2464, 1.97258, 1.73384, 1.52519, 1.34242,
    1.18197, 1.04086, 0.916546, 0.806832, 0.709875, 0.624101, 0.548176,
    0.480974, 0.421507, 0.368904, 0.322408, 0.281386, 0.245249, 0.213465,
    0.185549, 0.161072, 0.139644, 0.120913, 0.104568, 0.0903249, 0.0779269,
    0.0671493, 0.0577962, 0.0496902, 0.0426736, 0.0366093, 0.0313743,
    0.0268598, 0.0229699, 0.0196206, 0.0167399, 0.0142646, 0.0121397,
    0.0103181, 0.00875775, 0.00742226, 0.00628076, 0.00530519, 0.00447183,
    0.00376124, 0.00315632, 0.00264248, 0.00220738, 0.00184003, 0.00153095,
    0.00127204, 0.00105608, 0.000876652, 0.00072798, 0.00060492,
    0.000503201, 0.000419226, 0.000349896, 0.000292659, 0.000245421,
    0.000206394, 0.000174125, 0.000147441, 0.000125333, 0.000106985,
    9.173e-05, 7.90172e-05, 6.84172e-05, 5.95574e-05, 5.21183e-05,
    4.58348e-05, 4.05127e-05, 3.59987e-05, 3.21583e-05, 2.88718e-05,
    2.60322e-05, 2.35687e-05, 2.14263e-05, 1.95489e-05
  };

  static double tem[121] = {
    285.14, 279.34, 273.91, 268.3, 263.24, 256.55, 250.2, 242.82, 236.17,
    229.87, 225.04, 221.19, 218.85, 217.19, 216.2, 215.68, 215.42, 215.55,
    215.92, 216.4, 216.93, 217.45, 218, 218.68, 219.39, 220.25, 221.3,
    222.41, 223.88, 225.42, 227.2, 229.52, 231.89, 234.51, 236.85, 239.42,
    241.94, 244.57, 247.36, 250.32, 253.34, 255.82, 258.27, 260.39,
    262.03, 263.45, 264.2, 264.78, 264.67, 264.38, 263.24, 262.03, 260.02,
    258.09, 255.63, 253.28, 250.43, 247.81, 245.26, 242.77, 240.38,
    237.94, 235.79, 233.53, 231.5, 229.53, 227.6, 225.62, 223.77, 222.06,
    220.33, 218.69, 217.18, 215.64, 214.13, 212.52, 210.86, 209.25,
    207.49, 205.81, 204.11, 202.22, 200.32, 198.39, 195.92, 193.46,
    190.94, 188.31, 185.82, 183.57, 181.43, 179.74, 178.64, 178.1, 178.25,
    178.7, 179.41, 180.67, 182.31, 184.18, 186.6, 189.53, 192.66, 196.54,
    201.13, 205.93, 211.73, 217.86, 225, 233.53, 242.57, 252.14, 261.48,
    272.97, 285.26, 299.12, 312.2, 324.17, 338.34, 352.56, 365.28
  };
```

```
static double c2h2[121] = {
  1.352e-09, 2.83e-10, 1.269e-10, 6.926e-11, 4.346e-11, 2.909e-11,
  2.014e-11, 1.363e-11, 8.71e-12, 5.237e-12, 2.718e-12, 1.375e-12,
  5.786e-13, 2.16e-13, 7.317e-14, 2.551e-14, 1.055e-14, 4.758e-15,
  2.056e-15, 7.703e-16, 2.82e-16, 1.035e-16, 4.382e-17, 1.946e-17,
  9.638e-18, 5.2e-18, 2.811e-18, 1.494e-18, 7.925e-19, 4.213e-19,
  1.998e-19, 8.78e-20, 3.877e-20, 1.728e-20, 7.743e-21, 3.536e-21,
  1.623e-21, 7.508e-22, 3.508e-22, 1.65e-22, 7.837e-23, 3.733e-23,
  1.808e-23, 8.77e-24, 4.285e-24, 2.095e-24, 1.032e-24, 5.082e-25,
  2.506e-25, 1.236e-25, 6.088e-26, 2.996e-26, 1.465e-26, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
};

static double c2h6[121] = {
  2.667e-09, 2.02e-09, 1.658e-09, 1.404e-09, 1.234e-09, 1.109e-09,
  1.012e-09, 9.262e-10, 8.472e-10, 7.71e-10, 6.932e-10, 6.216e-10,
  5.503e-10, 4.87e-10, 4.342e-10, 3.861e-10, 3.347e-10, 2.772e-10,
  2.209e-10, 1.672e-10, 1.197e-10, 8.536e-11, 5.783e-11, 3.846e-11,
  2.495e-11, 1.592e-11, 1.017e-11, 6.327e-12, 3.895e-12, 2.403e-12,
  1.416e-12, 8.101e-13, 4.649e-13, 2.686e-13, 1.557e-13, 9.14e-14,
  5.386e-14, 3.19e-14, 1.903e-14, 1.14e-14, 6.875e-15, 4.154e-15,
  2.538e-15, 1.553e-15, 9.548e-16, 5.872e-16, 3.63e-16, 2.244e-16,
  1.388e-16, 8.587e-17, 5.308e-17, 3.279e-17, 2.017e-17, 1.238e-17,
  7.542e-18, 4.585e-18, 2.776e-18, 1.671e-18, 9.985e-19, 5.937e-19,
  3.518e-19, 2.07e-19, 1.215e-19, 7.06e-20, 4.097e-20, 2.37e-20,
  1.363e-20, 7.802e-21, 4.441e-21, 2.523e-21, 1.424e-21, 8.015e-22,
  4.497e-22, 2.505e-22, 1.391e-22, 7.691e-23, 4.238e-23, 2.331e-23,
  1.274e-23, 6.929e-24, 3.752e-24, 2.02e-24, 1.083e-24, 5.774e-25,
  3.041e-25, 1.593e-25, 8.308e-26, 4.299e-26, 2.195e-26, 1.112e-26,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0
};

static double ccl4[121] = {
  1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10,
  1.075e-10, 1.075e-10, 1.075e-10, 1.06e-10, 1.024e-10, 9.69e-11,
  8.93e-11, 8.078e-11, 7.213e-11, 6.307e-11, 5.383e-11, 4.49e-11,
  3.609e-11, 2.705e-11, 1.935e-11, 1.385e-11, 8.35e-12, 5.485e-12,
  3.853e-12, 2.22e-12, 5.875e-13, 3.445e-13, 1.015e-13, 6.075e-14,
  4.383e-14, 2.692e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14
};

static double ch4[121] = {
  1.864e-06, 1.835e-06, 1.819e-06, 1.805e-06, 1.796e-06, 1.788e-06,
  1.782e-06, 1.776e-06, 1.769e-06, 1.761e-06, 1.749e-06, 1.734e-06,
  1.716e-06, 1.692e-06, 1.654e-06, 1.61e-06, 1.567e-06, 1.502e-06,
  1.433e-06, 1.371e-06, 1.323e-06, 1.277e-06, 1.232e-06, 1.188e-06,
  1.147e-06, 1.108e-06, 1.07e-06, 1.027e-06, 9.854e-07, 9.416e-07,
  8.933e-07, 8.478e-07, 7.988e-07, 7.515e-07, 7.07e-07, 6.64e-07,
  6.239e-07, 5.864e-07, 5.512e-07, 5.184e-07, 4.87e-07, 4.571e-07,
  4.296e-07, 4.04e-07, 3.802e-07, 3.578e-07, 3.383e-07, 3.203e-07,
  3.032e-07, 2.889e-07, 2.76e-07, 2.635e-07, 2.519e-07, 2.409e-07,
  2.302e-07, 2.219e-07, 2.144e-07, 2.071e-07, 1.999e-07, 1.93e-07,
  1.862e-07, 1.795e-07, 1.731e-07, 1.668e-07, 1.607e-07, 1.548e-07,
  1.49e-07, 1.434e-07, 1.38e-07, 1.328e-07, 1.277e-07, 1.227e-07,
  1.18e-07, 1.134e-07, 1.089e-07, 1.046e-07, 1.004e-07, 9.635e-08,
  9.245e-08, 8.867e-08, 8.502e-08, 8.15e-08, 7.809e-08, 7.48e-08,
  7.159e-08, 6.849e-08, 6.55e-08, 6.262e-08, 5.98e-08, 5.708e-08,
  5.448e-08, 5.194e-08, 4.951e-08, 4.72e-08, 4.5e-08, 4.291e-08,
  4.093e-08, 3.905e-08, 3.729e-08, 3.563e-08, 3.408e-08, 3.265e-08,
  3.128e-08, 2.996e-08, 2.87e-08, 2.76e-08, 2.657e-08, 2.558e-08,
  2.467e-08, 2.385e-08, 2.307e-08, 2.234e-08, 2.168e-08, 2.108e-08,
  2.05e-08, 1.998e-08, 1.947e-08, 1.902e-08, 1.86e-08, 1.819e-08,
  1.782e-08
};

static double clo[121] = {
  7.419e-15, 1.061e-14, 1.518e-14, 2.195e-14, 3.175e-14, 4.666e-14,
  6.872e-14, 1.03e-13, 1.553e-13, 2.375e-13, 3.664e-13, 5.684e-13,
  8.915e-13, 1.402e-12, 2.269e-12, 4.125e-12, 7.501e-12, 1.257e-11,
  2.048e-11, 3.338e-11, 5.44e-11, 8.846e-11, 1.008e-10, 1.082e-10,
  1.157e-10, 1.232e-10, 1.312e-10, 1.539e-10, 1.822e-10, 2.118e-10,
  2.387e-10, 2.687e-10, 2.875e-10, 3.031e-10, 3.23e-10, 3.648e-10,
  4.117e-10, 4.477e-10, 4.633e-10, 4.794e-10, 4.95e-10, 5.104e-10,
  5.259e-10, 5.062e-10, 4.742e-10, 4.443e-10, 4.051e-10, 3.659e-10,
```

```
  3.305e-10, 2.911e-10, 2.54e-10, 2.215e-10, 1.927e-10, 1.675e-10,
  1.452e-10, 1.259e-10, 1.09e-10, 9.416e-11, 8.119e-11, 6.991e-11,
  6.015e-11, 5.163e-11, 4.43e-11, 3.789e-11, 3.24e-11, 2.769e-11,
  2.361e-11, 2.011e-11, 1.71e-11, 1.453e-11, 1.233e-11, 1.045e-11,
  8.851e-12, 7.48e-12, 6.316e-12, 5.326e-12, 4.487e-12, 3.778e-12,
  3.176e-12, 2.665e-12, 2.234e-12, 1.87e-12, 1.563e-12, 1.304e-12,
  1.085e-12, 9.007e-13, 7.468e-13, 6.179e-13, 5.092e-13, 4.188e-13,
  3.442e-13, 2.816e-13, 2.304e-13, 1.885e-13, 1.542e-13, 1.263e-13,
  1.035e-13, 8.5e-14, 7.004e-14, 5.783e-14, 4.795e-14, 4.007e-14,
  3.345e-14, 2.792e-14, 2.33e-14, 1.978e-14, 1.686e-14, 1.438e-14,
  1.234e-14, 1.07e-14, 9.312e-15, 8.131e-15, 7.164e-15, 6.367e-15,
  5.67e-15, 5.088e-15, 4.565e-15, 4.138e-15, 3.769e-15, 3.432e-15,
  3.148e-15
};

static double clono2[121] = {
  1.011e-13, 1.515e-13, 2.272e-13, 3.446e-13, 5.231e-13, 8.085e-13,
  1.253e-12, 1.979e-12, 3.149e-12, 5.092e-12, 8.312e-12, 1.366e-11,
  2.272e-11, 3.791e-11, 6.209e-11, 9.101e-11, 1.334e-10, 1.951e-10,
  2.853e-10, 3.94e-10, 4.771e-10, 5.771e-10, 6.675e-10, 7.665e-10,
  8.504e-10, 8.924e-10, 9.363e-10, 8.923e-10, 8.411e-10, 7.646e-10,
  6.525e-10, 5.576e-10, 4.398e-10, 3.403e-10, 2.612e-10, 1.915e-10,
  1.407e-10, 1.028e-10, 7.455e-11, 5.42e-11, 3.708e-11, 2.438e-11,
  1.618e-11, 1.075e-11, 7.17e-12, 4.784e-12, 3.205e-12, 2.147e-12,
  1.44e-12, 9.654e-13, 6.469e-13, 4.332e-13, 2.891e-13, 1.926e-13,
  1.274e-13, 8.422e-14, 5.547e-14, 3.636e-14, 2.368e-14, 1.536e-14,
  9.937e-15, 6.39e-15, 4.101e-15, 2.61e-15, 1.659e-15, 1.052e-15,
  6.638e-16, 4.172e-16, 2.61e-16, 1.63e-16, 1.013e-16, 6.275e-17,
  3.879e-17, 2.383e-17, 1.461e-17, 8.918e-18, 5.43e-18, 3.301e-18,
  1.997e-18, 1.203e-18, 7.216e-19, 4.311e-19, 2.564e-19, 1.519e-19,
  8.911e-20, 5.203e-20, 3.026e-20, 1.748e-20, 9.99e-21, 5.673e-21,
  3.215e-21, 1.799e-21, 1.006e-21, 5.628e-22, 3.146e-22, 1.766e-22,
  9.94e-23, 5.614e-23, 3.206e-23, 1.841e-23, 1.071e-23, 6.366e-24,
  3.776e-24, 2.238e-24, 1.326e-24, 8.253e-25, 5.201e-25, 3.279e-25,
  2.108e-25, 1.395e-25, 9.326e-26, 6.299e-26, 4.365e-26, 3.104e-26,
  2.219e-26, 1.621e-26, 1.185e-26, 8.92e-27, 6.804e-27, 5.191e-27,
  4.041e-27
};

static double co[121] = {
  1.907e-07, 1.553e-07, 1.362e-07, 1.216e-07, 1.114e-07, 1.036e-07,
  9.737e-08, 9.152e-08, 8.559e-08, 7.966e-08, 7.277e-08, 6.615e-08,
  5.884e-08, 5.22e-08, 4.699e-08, 4.284e-08, 3.776e-08, 3.274e-08,
  2.845e-08, 2.479e-08, 2.246e-08, 2.054e-08, 1.991e-08, 1.951e-08,
  1.94e-08, 2.009e-08, 2.1e-08, 2.201e-08, 2.322e-08, 2.45e-08,
  2.602e-08, 2.73e-08, 2.867e-08, 2.998e-08, 3.135e-08, 3.255e-08,
  3.352e-08, 3.426e-08, 3.484e-08, 3.53e-08, 3.593e-08, 3.671e-08,
  3.759e-08, 3.945e-08, 4.192e-08, 4.49e-08, 5.03e-08, 5.703e-08,
  6.538e-08, 7.878e-08, 9.644e-08, 1.196e-07, 1.498e-07, 1.904e-07,
  2.422e-07, 3.055e-07, 3.804e-07, 4.747e-07, 5.899e-07, 7.272e-07,
  8.91e-07, 1.071e-06, 1.296e-06, 1.546e-06, 1.823e-06, 2.135e-06,
  2.44e-06, 2.714e-06, 2.967e-06, 3.189e-06, 3.391e-06, 3.58e-06,
  3.773e-06, 4.022e-06, 4.346e-06, 4.749e-06, 5.199e-06, 5.668e-06,
  6.157e-06, 6.688e-06, 7.254e-06, 7.867e-06, 8.539e-06, 9.26e-06,
  1.009e-05, 1.119e-05, 1.228e-05, 1.365e-05, 1.506e-05, 1.641e-05,
  1.784e-05, 1.952e-05, 2.132e-05, 2.323e-05, 2.531e-05, 2.754e-05,
  3.047e-05, 3.459e-05, 3.922e-05, 4.439e-05, 4.825e-05, 5.077e-05,
  5.34e-05, 5.618e-05, 5.909e-05, 6.207e-05, 6.519e-05, 6.845e-05,
  6.819e-05, 6.726e-05, 6.622e-05, 6.512e-05, 6.671e-05, 6.862e-05,
  7.048e-05, 7.264e-05, 7.3e-05, 7.3e-05, 7.3e-05, 7.3e-05, 7.3e-05
};

static double cof2[121] = {
  7.5e-14, 1.055e-13, 1.485e-13, 2.111e-13, 3.001e-13, 4.333e-13,
  6.269e-13, 9.221e-13, 1.364e-12, 2.046e-12, 3.093e-12, 4.703e-12,
  7.225e-12, 1.113e-11, 1.66e-11, 2.088e-11, 2.626e-11, 3.433e-11,
  4.549e-11, 5.886e-11, 7.21e-11, 8.824e-11, 1.015e-10, 1.155e-10,
  1.288e-10, 1.388e-10, 1.497e-10, 1.554e-10, 1.606e-10, 1.639e-10,
  1.64e-10, 1.64e-10, 1.596e-10, 1.542e-10, 1.482e-10, 1.382e-10,
  1.289e-10, 1.198e-10, 1.109e-10, 1.026e-10, 9.484e-11, 8.75e-11,
  8.086e-11, 7.49e-11, 6.948e-11, 6.446e-11, 5.961e-11, 5.505e-11,
  5.085e-11, 4.586e-11, 4.1e-11, 3.665e-11, 3.235e-11, 2.842e-11,
  2.491e-11, 2.11e-11, 1.769e-11, 1.479e-11, 1.197e-11, 9.631e-12,
  7.74e-12, 6.201e-12, 4.963e-12, 3.956e-12, 3.151e-12, 2.507e-12,
  1.99e-12, 1.576e-12, 1.245e-12, 9.83e-13, 7.742e-13, 6.088e-13,
  4.782e-13, 3.745e-13, 2.929e-13, 2.286e-13, 1.782e-13, 1.388e-13,
  1.079e-13, 8.362e-14, 6.471e-14, 4.996e-14, 3.85e-14, 2.96e-14,
  2.265e-14, 1.729e-14, 1.317e-14, 9.998e-15, 7.549e-15, 5.683e-15,
  4.273e-15, 3.193e-15, 2.385e-15, 1.782e-15, 1.331e-15, 9.957e-16,
  7.461e-16, 5.601e-16, 4.228e-16, 3.201e-16, 2.438e-16, 1.878e-16,
  1.445e-16, 1.111e-16, 8.544e-17, 6.734e-17, 5.341e-17, 4.237e-17,
  3.394e-17, 2.759e-17, 2.254e-17, 1.851e-17, 1.54e-17, 1.297e-17,
  1.096e-17, 9.365e-18, 8e-18, 6.938e-18, 6.056e-18, 5.287e-18,
  4.662e-18
};

static double f11[121] = {
```

```
    2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10,
    2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.635e-10, 2.536e-10,
    2.44e-10, 2.348e-10, 2.258e-10, 2.153e-10, 2.046e-10, 1.929e-10,
    1.782e-10, 1.648e-10, 1.463e-10, 1.291e-10, 1.1e-10, 8.874e-11,
    7.165e-11, 5.201e-11, 3.744e-11, 2.577e-11, 1.64e-11, 1.048e-11,
    5.993e-12, 3.345e-12, 1.839e-12, 9.264e-13, 4.688e-13, 2.329e-13,
    1.129e-13, 5.505e-14, 2.825e-14, 1.492e-14, 7.997e-15, 5.384e-15,
    3.988e-15, 2.955e-15, 2.196e-15, 1.632e-15, 1.214e-15, 9.025e-16,
    6.708e-16, 4.984e-16, 3.693e-16, 2.733e-16, 2.013e-16, 1.481e-16,
    1.087e-16, 7.945e-17, 5.782e-17, 4.195e-17, 3.038e-17, 2.19e-17,
    1.577e-17, 1.128e-17, 8.063e-18, 5.753e-18, 4.09e-18, 2.899e-18,
    2.048e-18, 1.444e-18, 1.015e-18, 7.12e-19, 4.985e-19, 3.474e-19,
    2.417e-19, 1.677e-19, 1.161e-19, 8.029e-20, 5.533e-20, 3.799e-20,
    2.602e-20, 1.776e-20, 1.209e-20, 8.202e-21, 5.522e-21, 3.707e-21,
    2.48e-21, 1.652e-21, 1.091e-21, 7.174e-22, 4.709e-22, 3.063e-22,
    1.991e-22, 1.294e-22, 8.412e-23, 5.483e-23, 3.581e-23, 2.345e-23,
    1.548e-23, 1.027e-23, 6.869e-24, 4.673e-24, 3.173e-24, 2.153e-24,
    1.461e-24, 1.028e-24, 7.302e-25, 5.188e-25, 3.739e-25, 2.753e-25,
    2.043e-25, 1.528e-25, 1.164e-25, 9.041e-26, 7.051e-26, 5.587e-26,
    4.428e-26, 3.588e-26, 2.936e-26, 2.402e-26, 1.995e-26
  };

  static double f12[121] = {
    5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10,
    5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.429e-10, 5.291e-10,
    5.155e-10, 5.022e-10, 4.893e-10, 4.772e-10, 4.655e-10, 4.497e-10,
    4.249e-10, 4.015e-10, 3.632e-10, 3.261e-10, 2.858e-10, 2.408e-10,
    2.03e-10, 1.685e-10, 1.4e-10, 1.163e-10, 9.65e-11, 8.02e-11, 6.705e-11,
    5.624e-11, 4.764e-11, 4.249e-11, 3.792e-11, 3.315e-11, 2.819e-11,
    2.4e-11, 1.999e-11, 1.64e-11, 1.352e-11, 1.14e-11, 9.714e-12,
    8.28e-12, 7.176e-12, 6.251e-12, 5.446e-12, 4.72e-12, 4.081e-12,
    3.528e-12, 3.08e-12, 2.699e-12, 2.359e-12, 2.111e-12, 1.901e-12,
    1.709e-12, 1.534e-12, 1.376e-12, 1.233e-12, 1.103e-12, 9.869e-13,
    8.808e-13, 7.859e-13, 7.008e-13, 6.241e-13, 5.553e-13, 4.935e-13,
    4.383e-13, 3.889e-13, 3.447e-13, 3.054e-13, 2.702e-13, 2.389e-13,
    2.11e-13, 1.862e-13, 1.643e-13, 1.448e-13, 1.274e-13, 1.121e-13,
    9.844e-14, 8.638e-14, 7.572e-14, 6.62e-14, 5.782e-14, 5.045e-14,
    4.394e-14, 3.817e-14, 3.311e-14, 2.87e-14, 2.48e-14, 2.142e-14,
    1.851e-14, 1.599e-14, 1.383e-14, 1.196e-14, 1.036e-14, 9e-15,
    7.828e-15, 6.829e-15, 5.992e-15, 5.254e-15, 4.606e-15, 4.037e-15,
    3.583e-15, 3.19e-15, 2.841e-15, 2.542e-15, 2.291e-15, 2.07e-15,
    1.875e-15, 1.71e-15, 1.57e-15, 1.442e-15, 1.333e-15, 1.232e-15,
    1.147e-15, 1.071e-15, 1.001e-15, 9.396e-16
  };

  static double f14[121] = {
    9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11,
    9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 8.91e-11, 8.73e-11, 8.46e-11,
    8.19e-11, 7.92e-11, 7.74e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
    7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11
  };

  static double f22[121] = {
    1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10,
    1.4e-10, 1.4e-10, 1.4e-10, 1.372e-10, 1.317e-10, 1.235e-10, 1.153e-10,
    1.075e-10, 1.002e-10, 9.332e-11, 8.738e-11, 8.194e-11, 7.7e-11,
    7.165e-11, 6.753e-11, 6.341e-11, 5.971e-11, 5.6e-11, 5.229e-11,
    4.859e-11, 4.488e-11, 4.118e-11, 3.83e-11, 3.568e-11, 3.308e-11,
    3.047e-11, 2.82e-11, 2.594e-11, 2.409e-11, 2.237e-11, 2.065e-11,
    1.894e-11, 1.771e-11, 1.647e-11, 1.532e-11, 1.416e-11, 1.332e-11,
    1.246e-11, 1.161e-11, 1.087e-11, 1.017e-11, 9.471e-12, 8.853e-12,
    8.235e-12, 7.741e-12, 7.247e-12, 6.836e-12, 6.506e-12, 6.176e-12,
    5.913e-12, 5.65e-12, 5.419e-12, 5.221e-12, 5.024e-12, 4.859e-12,
    4.694e-12, 4.546e-12, 4.414e-12, 4.282e-12, 4.15e-12, 4.019e-12,
    3.903e-12, 3.805e-12, 3.706e-12, 3.607e-12, 3.508e-12, 3.41e-12,
    3.31e-12, 3.212e-12, 3.129e-12, 3.047e-12, 2.964e-12, 2.882e-12,
    2.8e-12, 2.734e-12, 2.668e-12, 2.602e-12, 2.537e-12, 2.471e-12,
    2.421e-12, 2.372e-12, 2.322e-12, 2.273e-12, 2.224e-12, 2.182e-12,
    2.141e-12, 2.1e-12, 2.059e-12, 2.018e-12, 1.977e-12, 1.935e-12,
    1.894e-12, 1.853e-12, 1.812e-12, 1.77e-12, 1.73e-12, 1.688e-12,
    1.647e-12, 1.606e-12, 1.565e-12, 1.524e-12, 1.483e-12, 1.441e-12,
    1.4e-12, 1.359e-12, 1.317e-12, 1.276e-12, 1.235e-12, 1.194e-12,
    1.153e-12, 1.112e-12, 1.071e-12, 1.029e-12, 9.883e-13
  };
```

```
static double h2o[121] = {
  0.01166, 0.008269, 0.005742, 0.003845, 0.00277, 0.001897, 0.001272,
  0.000827, 0.000539, 0.0003469, 0.0001579, 3.134e-05, 1.341e-05,
  6.764e-06, 4.498e-06, 3.703e-06, 3.724e-06, 3.899e-06, 4.002e-06,
  4.122e-06, 4.277e-06, 4.438e-06, 4.558e-06, 4.673e-06, 4.763e-06,
  4.809e-06, 4.856e-06, 4.936e-06, 5.021e-06, 5.114e-06, 5.222e-06,
  5.331e-06, 5.414e-06, 5.488e-06, 5.563e-06, 5.633e-06, 5.704e-06,
  5.767e-06, 5.819e-06, 5.872e-06, 5.914e-06, 5.949e-06, 5.984e-06,
  6.015e-06, 6.044e-06, 6.073e-06, 6.104e-06, 6.136e-06, 6.167e-06,
  6.189e-06, 6.208e-06, 6.226e-06, 6.212e-06, 6.185e-06, 6.158e-06,
  6.114e-06, 6.066e-06, 6.018e-06, 5.877e-06, 5.728e-06, 5.582e-06,
  5.437e-06, 5.296e-06, 5.156e-06, 5.02e-06, 4.886e-06, 4.754e-06,
  4.625e-06, 4.498e-06, 4.374e-06, 4.242e-06, 4.096e-06, 3.955e-06,
  3.817e-06, 3.683e-06, 3.491e-06, 3.204e-06, 2.94e-06, 2.696e-06,
  2.47e-06, 2.252e-06, 2.019e-06, 1.808e-06, 1.618e-06, 1.445e-06,
  1.285e-06, 1.105e-06, 9.489e-07, 8.121e-07, 6.938e-07, 5.924e-07,
  5.04e-07, 4.288e-07, 3.648e-07, 3.103e-07, 2.642e-07, 2.252e-07,
  1.921e-07, 1.643e-07, 1.408e-07, 1.211e-07, 1.048e-07, 9.063e-08,
  7.835e-08, 6.774e-08, 5.936e-08, 5.221e-08, 4.592e-08, 4.061e-08,
  3.62e-08, 3.236e-08, 2.902e-08, 2.62e-08, 2.383e-08, 2.171e-08,
  1.989e-08, 1.823e-08, 1.684e-08, 1.562e-08, 1.449e-08, 1.351e-08
};

static double h2o2[121] = {
  1.779e-10, 7.938e-10, 8.953e-10, 8.032e-10, 6.564e-10, 5.159e-10,
  4.003e-10, 3.026e-10, 2.222e-10, 1.58e-10, 1.044e-10, 6.605e-11,
  3.413e-11, 1.453e-11, 1.062e-11, 1.009e-11, 9.597e-12, 1.175e-11,
  1.572e-11, 2.091e-11, 2.746e-11, 3.603e-11, 4.791e-11, 6.387e-11,
  8.239e-11, 1.007e-10, 1.23e-10, 1.363e-10, 1.489e-10, 1.585e-10,
  1.608e-10, 1.632e-10, 1.576e-10, 1.502e-10, 1.423e-10, 1.302e-10,
  1.192e-10, 1.085e-10, 9.795e-11, 8.854e-11, 8.057e-11, 7.36e-11,
  6.736e-11, 6.362e-11, 6.087e-11, 5.825e-11, 5.623e-11, 5.443e-11,
  5.27e-11, 5.098e-11, 4.931e-11, 4.769e-11, 4.611e-11, 4.458e-11,
  4.308e-11, 4.102e-11, 3.887e-11, 3.682e-11, 3.521e-11, 3.369e-11,
  3.224e-11, 3.082e-11, 2.946e-11, 2.814e-11, 2.687e-11, 2.566e-11,
  2.449e-11, 2.336e-11, 2.227e-11, 2.123e-11, 2.023e-11, 1.927e-11,
  1.835e-11, 1.746e-11, 1.661e-11, 1.58e-11, 1.502e-11, 1.428e-11,
  1.357e-11, 1.289e-11, 1.224e-11, 1.161e-11, 1.102e-11, 1.045e-11,
  9.895e-12, 9.369e-12, 8.866e-12, 8.386e-12, 7.922e-12, 7.479e-12,
  7.06e-12, 6.656e-12, 6.274e-12, 5.914e-12, 5.575e-12, 5.257e-12,
  4.959e-12, 4.679e-12, 4.42e-12, 4.178e-12, 3.954e-12, 3.75e-12,
  3.557e-12, 3.372e-12, 3.198e-12, 3.047e-12, 2.908e-12, 2.775e-12,
  2.653e-12, 2.544e-12, 2.442e-12, 2.346e-12, 2.26e-12, 2.183e-12,
  2.11e-12, 2.044e-12, 1.98e-12, 1.924e-12, 1.871e-12, 1.821e-12,
  1.775e-12
};

static double hcn[121] = {
  5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10,
  5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.498e-10, 5.495e-10, 5.493e-10,
  5.49e-10, 5.488e-10, 4.717e-10, 3.946e-10, 3.174e-10, 2.4e-10,
  1.626e-10, 1.619e-10, 1.612e-10, 1.602e-10, 1.593e-10, 1.582e-10,
  1.572e-10, 1.56e-10, 1.549e-10, 1.539e-10, 1.53e-10, 1.519e-10,
  1.506e-10, 1.487e-10, 1.467e-10, 1.449e-10, 1.43e-10, 1.413e-10,
  1.397e-10, 1.382e-10, 1.368e-10, 1.354e-10, 1.337e-10, 1.315e-10,
  1.292e-10, 1.267e-10, 1.241e-10, 1.215e-10, 1.19e-10, 1.165e-10,
  1.141e-10, 1.118e-10, 1.096e-10, 1.072e-10, 1.047e-10, 1.021e-10,
  9.968e-11, 9.739e-11, 9.539e-11, 9.339e-11, 9.135e-11, 8.898e-11,
  8.664e-11, 8.439e-11, 8.249e-11, 8.075e-11, 7.904e-11, 7.735e-11,
  7.565e-11, 7.399e-11, 7.245e-11, 7.109e-11, 6.982e-11, 6.863e-11,
  6.755e-11, 6.657e-11, 6.587e-11, 6.527e-11, 6.476e-11, 6.428e-11,
  6.382e-11, 6.343e-11, 6.307e-11, 6.272e-11, 6.238e-11, 6.205e-11,
  6.17e-11, 6.137e-11, 6.102e-11, 6.072e-11, 6.046e-11, 6.03e-11,
  6.018e-11, 6.01e-11, 6.001e-11, 5.992e-11, 5.984e-11, 5.975e-11,
  5.967e-11, 5.958e-11, 5.95e-11, 5.941e-11, 5.933e-11, 5.925e-11,
  5.916e-11, 5.908e-11, 5.899e-11, 5.891e-11, 5.883e-11, 5.874e-11,
  5.866e-11, 5.858e-11, 5.85e-11, 5.841e-11, 5.833e-11, 5.825e-11,
  5.817e-11, 5.808e-11, 5.8e-11, 5.792e-11, 5.784e-11
};

static double hno3[121] = {
  1.809e-10, 7.234e-10, 5.899e-10, 4.342e-10, 3.277e-10, 2.661e-10,
  2.35e-10, 2.267e-10, 2.389e-10, 2.651e-10, 3.255e-10, 4.099e-10,
  5.42e-10, 6.978e-10, 8.807e-10, 1.112e-09, 1.405e-09, 2.04e-09,
  3.111e-09, 4.5e-09, 5.762e-09, 7.37e-09, 7.852e-09, 8.109e-09,
  8.067e-09, 7.554e-09, 7.076e-09, 6.268e-09, 5.524e-09, 4.749e-09,
  3.909e-09, 3.223e-09, 2.517e-09, 1.942e-09, 1.493e-09, 1.122e-09,
  8.449e-10, 6.361e-10, 4.787e-10, 3.611e-10, 2.804e-10, 2.215e-10,
  1.758e-10, 1.441e-10, 1.197e-10, 9.953e-11, 8.505e-11, 7.334e-11,
  6.325e-11, 5.625e-11, 5.058e-11, 4.548e-11, 4.122e-11, 3.748e-11,
  3.402e-11, 3.088e-11, 2.8e-11, 2.536e-11, 2.293e-11, 2.072e-11,
  1.871e-11, 1.687e-11, 1.52e-11, 1.368e-11, 1.23e-11, 1.105e-11,
  9.922e-12, 8.898e-12, 7.972e-12, 7.139e-12, 6.385e-12, 5.708e-12,
  5.099e-12, 4.549e-12, 4.056e-12, 3.613e-12, 3.216e-12, 2.862e-12,
  2.544e-12, 2.259e-12, 2.004e-12, 1.776e-12, 1.572e-12, 1.391e-12,
  1.227e-12, 1.082e-12, 9.528e-13, 8.379e-13, 7.349e-13, 6.436e-13,
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    5.634e-13, 4.917e-13, 4.291e-13, 3.745e-13, 3.267e-13, 2.854e-13,
    2.494e-13, 2.181e-13, 1.913e-13, 1.68e-13, 1.479e-13, 1.31e-13,
    1.159e-13, 1.025e-13, 9.067e-14, 8.113e-14, 7.281e-14, 6.535e-14,
    5.892e-14, 5.348e-14, 4.867e-14, 4.439e-14, 4.073e-14, 3.76e-14,
    3.476e-14, 3.229e-14, 3e-14, 2.807e-14, 2.635e-14, 2.473e-14,
    2.332e-14
  };

  static double hno4[121] = {
    6.118e-12, 3.594e-12, 2.807e-12, 3.04e-12, 4.458e-12, 7.986e-12,
    1.509e-11, 2.661e-11, 3.738e-11, 4.652e-11, 4.429e-11, 3.992e-11,
    3.347e-11, 3.005e-11, 3.173e-11, 4.055e-11, 5.812e-11, 8.489e-11,
    1.19e-10, 1.482e-10, 1.766e-10, 2.103e-10, 2.35e-10, 2.598e-10,
    2.801e-10, 2.899e-10, 3e-10, 2.817e-10, 2.617e-10, 2.332e-10,
    1.933e-10, 1.605e-10, 1.232e-10, 9.285e-11, 6.941e-11, 4.951e-11,
    3.539e-11, 2.402e-11, 1.522e-11, 9.676e-12, 6.056e-12, 3.745e-12,
    2.34e-12, 1.463e-12, 9.186e-13, 5.769e-13, 3.322e-13, 1.853e-13,
    1.035e-13, 7.173e-14, 5.382e-14, 4.036e-14, 3.401e-14, 2.997e-14,
    2.635e-14, 2.316e-14, 2.034e-14, 1.783e-14, 1.56e-14, 1.363e-14,
    1.19e-14, 1.037e-14, 9.032e-15, 7.846e-15, 6.813e-15, 5.912e-15,
    5.121e-15, 4.431e-15, 3.829e-15, 3.306e-15, 2.851e-15, 2.456e-15,
    2.114e-15, 1.816e-15, 1.559e-15, 1.337e-15, 1.146e-15, 9.811e-16,
    8.389e-16, 7.162e-16, 6.109e-16, 5.203e-16, 4.425e-16, 3.76e-16,
    3.184e-16, 2.692e-16, 2.274e-16, 1.917e-16, 1.61e-16, 1.35e-16,
    1.131e-16, 9.437e-17, 7.874e-17, 6.57e-17, 5.481e-17, 4.579e-17,
    3.828e-17, 3.204e-17, 2.691e-17, 2.264e-17, 1.912e-17, 1.626e-17,
    1.382e-17, 1.174e-17, 9.972e-18, 8.603e-18, 7.45e-18, 6.453e-18,
    5.623e-18, 4.944e-18, 4.361e-18, 3.859e-18, 3.443e-18, 3.096e-18,
    2.788e-18, 2.528e-18, 2.293e-18, 2.099e-18, 1.929e-18, 1.773e-18,
    1.64e-18
  };

  static double hocl[121] = {
    1.056e-12, 1.194e-12, 1.35e-12, 1.531e-12, 1.737e-12, 1.982e-12,
    2.263e-12, 2.599e-12, 2.991e-12, 3.459e-12, 4.012e-12, 4.662e-12,
    5.438e-12, 6.35e-12, 7.425e-12, 8.686e-12, 1.016e-11, 1.188e-11,
    1.389e-11, 1.659e-11, 2.087e-11, 2.621e-11, 3.265e-11, 4.064e-11,
    4.859e-11, 5.441e-11, 6.09e-11, 6.373e-11, 6.611e-11, 6.94e-11,
    7.44e-11, 7.97e-11, 8.775e-11, 9.722e-11, 1.064e-10, 1.089e-10,
    1.114e-10, 1.106e-10, 1.053e-10, 1.004e-10, 9.006e-11, 7.778e-11,
    6.739e-11, 5.636e-11, 4.655e-11, 3.845e-11, 3.042e-11, 2.368e-11,
    1.845e-11, 1.442e-11, 1.127e-11, 8.814e-12, 6.544e-12, 4.763e-12,
    3.449e-12, 2.612e-12, 1.999e-12, 1.526e-12, 1.16e-12, 8.793e-13,
    6.655e-13, 5.017e-13, 3.778e-13, 2.829e-13, 2.117e-13, 1.582e-13,
    1.178e-13, 8.755e-14, 6.486e-14, 4.799e-14, 3.54e-14, 2.606e-14,
    1.916e-14, 1.403e-14, 1.026e-14, 7.48e-15, 5.446e-15, 3.961e-15,
    2.872e-15, 2.076e-15, 1.498e-15, 1.077e-15, 7.726e-16, 5.528e-16,
    3.929e-16, 2.785e-16, 1.969e-16, 1.386e-16, 9.69e-17, 6.747e-17,
    4.692e-17, 3.236e-17, 2.232e-17, 1.539e-17, 1.061e-17, 7.332e-18,
    5.076e-18, 3.522e-18, 2.461e-18, 1.726e-18, 1.22e-18, 8.75e-19,
    6.264e-19, 4.482e-19, 3.207e-19, 2.368e-19, 1.762e-19, 1.312e-19,
    9.891e-20, 7.595e-20, 5.87e-20, 4.567e-20, 3.612e-20, 2.904e-20,
    2.343e-20, 1.917e-20, 1.568e-20, 1.308e-20, 1.1e-20, 9.25e-21,
    7.881e-21
  };

  static double n2o[121] = {
    3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07,
    3.17e-07, 3.17e-07, 3.17e-07, 3.124e-07, 3.077e-07, 3.03e-07,
    2.984e-07, 2.938e-07, 2.892e-07, 2.847e-07, 2.779e-07, 2.705e-07,
    2.631e-07, 2.557e-07, 2.484e-07, 2.345e-07, 2.201e-07, 2.01e-07,
    1.754e-07, 1.532e-07, 1.329e-07, 1.154e-07, 1.003e-07, 8.735e-08,
    7.617e-08, 6.512e-08, 5.547e-08, 4.709e-08, 3.915e-08, 3.259e-08,
    2.738e-08, 2.327e-08, 1.98e-08, 1.711e-08, 1.493e-08, 1.306e-08,
    1.165e-08, 1.049e-08, 9.439e-09, 8.375e-09, 7.391e-09, 6.525e-09,
    5.759e-09, 5.083e-09, 4.485e-09, 3.953e-09, 3.601e-09, 3.27e-09,
    2.975e-09, 2.757e-09, 2.556e-09, 2.37e-09, 2.195e-09, 2.032e-09,
    1.912e-09, 1.79e-09, 1.679e-09, 1.572e-09, 1.482e-09, 1.402e-09,
    1.326e-09, 1.254e-09, 1.187e-09, 1.127e-09, 1.071e-09, 1.02e-09,
    9.673e-10, 9.193e-10, 8.752e-10, 8.379e-10, 8.017e-10, 7.66e-10,
    7.319e-10, 7.004e-10, 6.721e-10, 6.459e-10, 6.199e-10, 5.942e-10,
    5.703e-10, 5.488e-10, 5.283e-10, 5.082e-10, 4.877e-10, 4.696e-10,
    4.52e-10, 4.355e-10, 4.198e-10, 4.039e-10, 3.888e-10, 3.754e-10,
    3.624e-10, 3.499e-10, 3.381e-10, 3.267e-10, 3.163e-10, 3.058e-10,
    2.959e-10, 2.864e-10, 2.77e-10, 2.686e-10, 2.604e-10, 2.534e-10,
    2.462e-10, 2.386e-10, 2.318e-10, 2.247e-10, 2.189e-10, 2.133e-10,
    2.071e-10, 2.014e-10, 1.955e-10, 1.908e-10, 1.86e-10, 1.817e-10
  };

  static double n2o5[121] = {
    1.231e-11, 3.035e-12, 1.702e-12, 9.877e-13, 8.081e-13, 9.039e-13,
    1.169e-12, 1.474e-12, 1.651e-12, 1.795e-12, 1.998e-12, 2.543e-12,
    4.398e-12, 7.698e-12, 1.28e-11, 2.131e-11, 3.548e-11, 5.894e-11,
    7.645e-11, 1.089e-10, 1.391e-10, 1.886e-10, 2.386e-10, 2.986e-10,
    3.487e-10, 3.994e-10, 4.5e-10, 4.6e-10, 4.591e-10, 4.1e-10, 3.488e-10,
    2.846e-10, 2.287e-10, 1.696e-10, 1.011e-10, 6.428e-11, 4.324e-11,
    2.225e-11, 6.214e-12, 3.608e-12, 8.793e-13, 4.491e-13, 1.04e-13,
```

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    6.1e-14, 3.436e-14, 6.671e-15, 1.171e-15, 5.848e-16, 1.212e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
    1e-16, 1e-16
  };

  static double nh3[121] = {
    1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10,
    1e-10, 1e-10, 1e-10, 1e-10, 9.444e-11, 8.488e-11, 7.241e-11, 5.785e-11,
    4.178e-11, 3.018e-11, 2.18e-11, 1.574e-11, 1.137e-11, 8.211e-12,
    5.973e-12, 4.327e-12, 3.118e-12, 2.234e-12, 1.573e-12, 1.04e-12,
    6.762e-13, 4.202e-13, 2.406e-13, 1.335e-13, 6.938e-14, 3.105e-14,
    1.609e-14, 1.033e-14, 6.432e-15, 4.031e-15, 2.555e-15, 1.656e-15,
    1.115e-15, 7.904e-16, 5.63e-16, 4.048e-16, 2.876e-16, 2.004e-16,
    1.356e-16, 9.237e-17, 6.235e-17, 4.223e-17, 3.009e-17, 2.328e-17,
    2.002e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
    1.914e-17
  };

  static double no[121] = {
    2.586e-10, 4.143e-11, 1.566e-11, 9.591e-12, 8.088e-12, 8.462e-12,
    1.013e-11, 1.328e-11, 1.855e-11, 2.678e-11, 3.926e-11, 5.464e-11,
    7.012e-11, 8.912e-11, 1.127e-10, 1.347e-10, 1.498e-10, 1.544e-10,
    1.602e-10, 1.824e-10, 2.078e-10, 2.366e-10, 2.691e-10, 5.141e-10,
    8.259e-10, 1.254e-09, 1.849e-09, 2.473e-09, 3.294e-09, 4.16e-09,
    5.095e-09, 6.11e-09, 6.93e-09, 7.888e-09, 8.903e-09, 9.713e-09,
    1.052e-08, 1.115e-08, 1.173e-08, 1.21e-08, 1.228e-08, 1.239e-08,
    1.231e-08, 1.213e-08, 1.192e-08, 1.138e-08, 1.085e-08, 1.008e-08,
    9.224e-09, 8.389e-09, 7.262e-09, 6.278e-09, 5.335e-09, 4.388e-09,
    3.589e-09, 2.761e-09, 2.129e-09, 1.633e-09, 1.243e-09, 9.681e-10,
    8.355e-10, 7.665e-10, 7.442e-10, 8.584e-10, 9.732e-10, 1.063e-09,
    1.163e-09, 1.286e-09, 1.472e-09, 1.707e-09, 2.032e-09, 2.474e-09,
    2.977e-09, 3.506e-09, 4.102e-09, 5.013e-09, 6.493e-09, 8.414e-09,
    1.077e-08, 1.367e-08, 1.777e-08, 2.625e-08, 3.926e-08, 5.545e-08,
    7.195e-08, 9.464e-08, 1.404e-07, 2.183e-07, 3.329e-07, 4.535e-07,
    6.158e-07, 8.187e-07, 1.075e-06, 1.422e-06, 1.979e-06, 2.71e-06,
    3.58e-06, 4.573e-06, 5.951e-06, 7.999e-06, 1.072e-05, 1.372e-05,
    1.697e-05, 2.112e-05, 2.643e-05, 3.288e-05, 3.994e-05, 4.794e-05,
    5.606e-05, 6.383e-05, 7.286e-05, 8.156e-05, 8.883e-05, 9.469e-05,
    9.848e-05, 0.0001023, 0.0001066, 0.0001115, 0.0001145, 0.0001142,
    0.0001133
  };

  static double no2[121] = {
    3.036e-09, 2.945e-10, 9.982e-11, 5.069e-11, 3.485e-11, 2.982e-11,
    2.947e-11, 3.164e-11, 3.714e-11, 4.586e-11, 6.164e-11, 8.041e-11,
    9.982e-11, 1.283e-10, 1.73e-10, 2.56e-10, 3.909e-10, 5.959e-10,
    9.081e-10, 1.384e-09, 1.788e-09, 2.189e-09, 2.686e-09, 3.091e-09,
    3.49e-09, 3.796e-09, 4.2e-09, 5.103e-09, 6.005e-09, 6.3e-09, 6.706e-09,
    7.07e-09, 7.434e-09, 7.663e-09, 7.788e-09, 7.8e-09, 7.597e-09,
    7.482e-09, 7.227e-09, 6.403e-09, 5.585e-09, 4.606e-09, 3.703e-09,
    2.984e-09, 2.183e-09, 1.48e-09, 8.441e-10, 5.994e-10, 3.799e-10,
    2.751e-10, 1.927e-10, 1.507e-10, 1.102e-10, 6.971e-11, 5.839e-11,
    3.904e-11, 3.087e-11, 2.176e-11, 1.464e-11, 1.209e-11, 8.497e-12,
    6.477e-12, 4.371e-12, 2.914e-12, 2.424e-12, 1.753e-12, 1.35e-12,
    9.417e-13, 6.622e-13, 5.148e-13, 3.841e-13, 3.446e-13, 3.01e-13,
    2.551e-13, 2.151e-13, 1.829e-13, 1.64e-13, 1.475e-13, 1.352e-13,
    1.155e-13, 9.963e-14, 9.771e-14, 9.577e-14, 9.384e-14, 9.186e-14,
    9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
    9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
    9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
    9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14
  };

  static double o3[121] = {
    2.218e-08, 3.394e-08, 3.869e-08, 4.219e-08, 4.501e-08, 4.778e-08,
    5.067e-08, 5.402e-08, 5.872e-08, 6.521e-08, 7.709e-08, 9.461e-08,
    1.269e-07, 1.853e-07, 2.723e-07, 3.964e-07, 5.773e-07, 8.2e-07,
    1.155e-06, 1.59e-06, 2.076e-06, 2.706e-06, 3.249e-06, 3.848e-06,
    4.459e-06, 4.986e-06, 5.573e-06, 5.958e-06, 6.328e-06, 6.661e-06,
    6.9e-06, 7.146e-06, 7.276e-06, 7.374e-06, 7.447e-06, 7.383e-06,
    7.321e-06, 7.161e-06, 6.879e-06, 6.611e-06, 6.216e-06, 5.765e-06,
```

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    5.355e-06, 4.905e-06, 4.471e-06, 4.075e-06, 3.728e-06, 3.413e-06,
    3.125e-06, 2.856e-06, 2.607e-06, 2.379e-06, 2.17e-06, 1.978e-06,
    1.8e-06, 1.646e-06, 1.506e-06, 1.376e-06, 1.233e-06, 1.102e-06,
    9.839e-07, 8.771e-07, 7.814e-07, 6.947e-07, 6.102e-07, 5.228e-07,
    4.509e-07, 3.922e-07, 3.501e-07, 3.183e-07, 2.909e-07, 2.686e-07,
    2.476e-07, 2.284e-07, 2.109e-07, 2.003e-07, 2.013e-07, 2.022e-07,
    2.032e-07, 2.042e-07, 2.097e-07, 2.361e-07, 2.656e-07, 2.989e-07,
    3.37e-07, 3.826e-07, 4.489e-07, 5.26e-07, 6.189e-07, 7.312e-07,
    8.496e-07, 8.444e-07, 8.392e-07, 8.339e-07, 8.286e-07, 8.234e-07,
    8.181e-07, 8.129e-07, 8.077e-07, 8.026e-07, 6.918e-07, 5.176e-07,
    3.865e-07, 2.885e-07, 2.156e-07, 1.619e-07, 1.219e-07, 9.161e-08,
    6.972e-08, 5.399e-08, 3.498e-08, 2.111e-08, 1.322e-08, 8.482e-09,
    5.527e-09, 3.423e-09, 2.071e-09, 1.314e-09, 8.529e-10, 5.503e-10,
    3.665e-10
  };

  static double ocs[121] = {
    6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 5.997e-10,
    5.989e-10, 5.881e-10, 5.765e-10, 5.433e-10, 5.074e-10, 4.567e-10,
    4.067e-10, 3.601e-10, 3.093e-10, 2.619e-10, 2.232e-10, 1.805e-10,
    1.46e-10, 1.187e-10, 8.03e-11, 5.435e-11, 3.686e-11, 2.217e-11,
    1.341e-11, 8.756e-12, 4.511e-12, 2.37e-12, 1.264e-12, 8.28e-13,
    5.263e-13, 3.209e-13, 1.717e-13, 9.068e-14, 4.709e-14, 2.389e-14,
    1.236e-14, 1.127e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
    1.091e-14, 1.091e-14, 1.091e-14
  };

  static double sf6[121] = {
    4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12,
    4.103e-12, 4.103e-12, 4.103e-12, 4.087e-12, 4.064e-12, 4.023e-12,
    3.988e-12, 3.941e-12, 3.884e-12, 3.755e-12, 3.622e-12, 3.484e-12,
    3.32e-12, 3.144e-12, 2.978e-12, 2.811e-12, 2.653e-12, 2.489e-12,
    2.332e-12, 2.199e-12, 2.089e-12, 2.013e-12, 1.953e-12, 1.898e-12,
    1.859e-12, 1.826e-12, 1.798e-12, 1.776e-12, 1.757e-12, 1.742e-12,
    1.728e-12, 1.717e-12, 1.707e-12, 1.698e-12, 1.691e-12, 1.685e-12,
    1.679e-12, 1.675e-12, 1.671e-12, 1.668e-12, 1.665e-12, 1.663e-12,
    1.661e-12, 1.659e-12, 1.658e-12, 1.657e-12, 1.656e-12, 1.655e-12,
    1.654e-12, 1.653e-12, 1.653e-12, 1.652e-12, 1.652e-12, 1.652e-12,
    1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12,
    1.651e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
    1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12
  };

  static double so2[121] = {
    1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10,
    1e-10, 1e-10, 9.867e-11, 9.537e-11, 9e-11, 8.404e-11, 7.799e-11,
    7.205e-11, 6.616e-11, 6.036e-11, 5.475e-11, 5.007e-11, 4.638e-11,
    4.346e-11, 4.055e-11, 3.763e-11, 3.471e-11, 3.186e-11, 2.905e-11,
    2.631e-11, 2.358e-11, 2.415e-11, 2.949e-11, 3.952e-11, 5.155e-11,
    6.76e-11, 8.741e-11, 1.099e-10, 1.278e-10, 1.414e-10, 1.512e-10,
    1.607e-10, 1.699e-10, 1.774e-10, 1.832e-10, 1.871e-10, 1.907e-10,
    1.943e-10, 1.974e-10, 1.993e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
    2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10
  };

  static int ig_co2 = -999;

  double *q[NG] = { NULL };

  /* Find emitter index of CO2... */
  if (ig_co2 == -999)
    ig_co2 = find_emitter(ctl, "CO2");

```

```
  /* Identify variable... */
  for (int ig = 0; ig < ctl->ng; ig++) {
    q[ig] = NULL;
    if (strcasecmp(ctl->emitter[ig], "C2H2") == 0)
      q[ig] = c2h2;
    if (strcasecmp(ctl->emitter[ig], "C2H6") == 0)
      q[ig] = c2h6;
    if (strcasecmp(ctl->emitter[ig], "CCl4") == 0)
      q[ig] = ccl4;
    if (strcasecmp(ctl->emitter[ig], "CH4") == 0)
      q[ig] = ch4;
    if (strcasecmp(ctl->emitter[ig], "ClO") == 0)
      q[ig] = clo;
    if (strcasecmp(ctl->emitter[ig], "ClONO2") == 0)
      q[ig] = clono2;
    if (strcasecmp(ctl->emitter[ig], "CO") == 0)
      q[ig] = co;
    if (strcasecmp(ctl->emitter[ig], "COF2") == 0)
      q[ig] = cof2;
    if (strcasecmp(ctl->emitter[ig], "F11") == 0)
      q[ig] = f11;
    if (strcasecmp(ctl->emitter[ig], "F12") == 0)
      q[ig] = f12;
    if (strcasecmp(ctl->emitter[ig], "F14") == 0)
      q[ig] = f14;
    if (strcasecmp(ctl->emitter[ig], "F22") == 0)
      q[ig] = f22;
    if (strcasecmp(ctl->emitter[ig], "H2O") == 0)
      q[ig] = h2o;
    if (strcasecmp(ctl->emitter[ig], "H2O2") == 0)
      q[ig] = h2o2;
    if (strcasecmp(ctl->emitter[ig], "HCN") == 0)
      q[ig] = hcn;
    if (strcasecmp(ctl->emitter[ig], "HNO3") == 0)
      q[ig] = hno3;
    if (strcasecmp(ctl->emitter[ig], "HNO4") == 0)
      q[ig] = hno4;
    if (strcasecmp(ctl->emitter[ig], "HOCl") == 0)
      q[ig] = hocl;
    if (strcasecmp(ctl->emitter[ig], "N2O") == 0)
      q[ig] = n2o;
    if (strcasecmp(ctl->emitter[ig], "N2O5") == 0)
      q[ig] = n2o5;
    if (strcasecmp(ctl->emitter[ig], "NH3") == 0)
      q[ig] = nh3;
    if (strcasecmp(ctl->emitter[ig], "NO") == 0)
      q[ig] = no;
    if (strcasecmp(ctl->emitter[ig], "NO2") == 0)
      q[ig] = no2;
    if (strcasecmp(ctl->emitter[ig], "O3") == 0)
      q[ig] = o3;
    if (strcasecmp(ctl->emitter[ig], "OCS") == 0)
      q[ig] = ocs;
    if (strcasecmp(ctl->emitter[ig], "SF6") == 0)
      q[ig] = sf6;
    if (strcasecmp(ctl->emitter[ig], "SO2") == 0)
      q[ig] = so2;
  }

  /* Loop over atmospheric data points... */
  for (int ip = 0; ip < atm->np; ip++) {

    /* Get altitude index... */
    int iz = locate_reg(z, 121, atm->z[ip]);

    /* Interpolate pressure... */
    atm->p[ip] = EXP(z[iz], pre[iz], z[iz + 1], pre[iz + 1], atm->z[ip]);

    /* Interpolate temperature... */
    atm->t[ip] = LIN(z[iz], tem[iz], z[iz + 1], tem[iz + 1], atm->z[ip]);

    /* Interpolate trace gases... */
    for (int ig = 0; ig < ctl->ng; ig++)
      if (q[ig] != NULL)
        atm->q[ig][ip] =
          LIN(z[iz], q[ig][iz], z[iz + 1], q[ig][iz + 1], atm->z[ip]);
      else
        atm->q[ig][ip] = 0;

    /* Set CO2... */
    if (ig_co2 >= 0)
      atm->q[ig_co2][ip] =
        371.789948e-6 + 2.026214e-6 * (atm->time[ip] - 63158400.) / 31557600.;

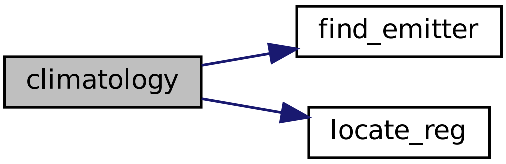
    /* Set extinction to zero... */
    for (int iw = 0; iw < ctl->nw; iw++)
      atm->k[iw][ip] = 0;
```

```

    /* Set cloud layer... */
    atm->clz = atm->cldz = 0;
    for (int icl = 0; icl < ctl->ncl; icl++)
      atm->clk[icl] = 0;

    /* Set surface layer... */
    atm->sfz = atm->sfp = atm->sft = 0;
    for (int isf = 0; isf < ctl->nsf; isf++)
      atm->sfeps[isf] = 1;
  }
}
```

Here is the call graph for this function:



5.17.2.6 ctmco2()

```
double ctmco2 (
    double nu,
    double p,
    double t,
    double u )
```

Compute carbon dioxide continuum (optical depth).

Definition at line 897 of file jurassic.c.

```
                 {

  static double co2296[2001] = { 9.3388e-5, 9.7711e-5, 1.0224e-4, 1.0697e-4,
    1.1193e-4, 1.1712e-4, 1.2255e-4, 1.2824e-4, 1.3419e-4, 1.4043e-4,
    1.4695e-4, 1.5378e-4, 1.6094e-4, 1.6842e-4, 1.7626e-4, 1.8447e-4,
    1.9307e-4, 2.0207e-4, 2.1149e-4, 2.2136e-4, 2.3169e-4, 2.4251e-4,
    2.5384e-4, 2.657e-4, 2.7813e-4, 2.9114e-4, 3.0477e-4, 3.1904e-4,
    3.3399e-4, 3.4965e-4, 3.6604e-4, 3.8322e-4, 4.0121e-4, 4.2006e-4,
    4.398e-4, 4.6047e-4, 4.8214e-4, 5.0483e-4, 5.286e-4, 5.535e-4,
    5.7959e-4, 6.0693e-4, 6.3557e-4, 6.6558e-4, 6.9702e-4, 7.2996e-4,
    7.6449e-4, 8.0066e-4, 8.3856e-4, 8.7829e-4, 9.1991e-4, 9.6354e-4,
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01731     .12584
01732   };
01733
01734   /* Get CO2 continuum absorption... */
01735   double xw = nu / 2 + 1;
01736   if (xw >= 1 && xw < 2001) {
01737     int iw = (int) xw;
01738     double dw = xw - iw;
01739     double ew = 1 - dw;
01740     double cw296 = ew * co2296[iw - 1] + dw * co2296[iw];
01741     double cw260 = ew * co2260[iw - 1] + dw * co2260[iw];
01742     double cw230 = ew * co2230[iw - 1] + dw * co2230[iw];
01743     double dt230 = t - 230;
01744     double dt260 = t - 260;
01745     double dt296 = t - 296;
01746     double ctw = dt260 * 5.050505e-4 * dt296 * cw230 - dt230 * 9.259259e-4
01747       * dt296 * cw260 + dt230 * 4.208754e-4 * dt260 * cw296;
01748     return u / NA / 1000 * p / P0 * ctw;
01749   } else
01750     return 0;
01751 }
```

5.17.2.7 ctmh2o()

```
double ctmh2o (
        double nu,
        double p,
        double t,
        double q,
        double u )
```

Compute water vapor continuum (optical depth).

Definition at line 1755 of file jurassic.c.

```
01760                 {
01761
01762   static double h2o296[2001] = { .17, .1695, .172, .168, .1687, .1624, .1606,
01763     .1508, .1447, .1344, .1214, .1133, .1009, .09217, .08297, .06989,
01764     .06513, .05469, .05056, .04417, .03779, .03484, .02994, .0272,
01765     .02325, .02063, .01818, .01592, .01405, .01251, .0108, .009647,
01766     .008424, .007519, .006555, .00588, .005136, .004511, .003989,
01767     .003509, .003114, .00274, .002446, .002144, .001895, .001676,
01768     .001486, .001312, .001164, .001031, 9.129e-4, 8.106e-4, 7.213e-4,
01769     6.4e-4, 5.687e-4, 5.063e-4, 4.511e-4, 4.029e-4, 3.596e-4,
01770     3.22e-4, 2.889e-4, 2.597e-4, 2.337e-4, 2.108e-4, 1.907e-4,
01771     1.728e-4, 1.57e-4, 1.43e-4, 1.305e-4, 1.195e-4, 1.097e-4,
01772     1.009e-4, 9.307e-5, 8.604e-5, 7.971e-5, 7.407e-5, 6.896e-5,
01773     6.433e-5, 6.013e-5, 5.631e-5, 5.283e-5, 4.963e-5, 4.669e-5,
01774     4.398e-5, 4.148e-5, 3.917e-5, 3.702e-5, 3.502e-5, 3.316e-5,
01775     3.142e-5, 2.978e-5, 2.825e-5, 2.681e-5, 2.546e-5, 2.419e-5,
01776     2.299e-5, 2.186e-5, 2.079e-5, 1.979e-5, 1.884e-5, 1.795e-5,
01777     1.711e-5, 1.633e-5, 1.559e-5, 1.49e-5, 1.426e-5, 1.367e-5,
01778     1.312e-5, 1.263e-5, 1.218e-5, 1.178e-5, 1.143e-5, 1.112e-5,
01779     1.088e-5, 1.07e-5, 1.057e-5, 1.05e-5, 1.051e-5, 1.059e-5,
01780     1.076e-5, 1.1e-5, 1.133e-5, 1.18e-5, 1.237e-5, 1.308e-5,
01781     1.393e-5, 1.483e-5, 1.614e-5, 1.758e-5, 1.93e-5, 2.123e-5,
01782     2.346e-5, 2.647e-5, 2.93e-5, 3.279e-5, 3.745e-5, 4.152e-5,
01783     4.813e-5, 5.477e-5, 6.203e-5, 7.331e-5, 8.056e-5, 9.882e-5,
01784     1.05e-4, 1.21e-4, 1.341e-4, 1.572e-4, 1.698e-4, 1.968e-4,
01785     2.175e-4, 2.431e-4, 2.735e-4, 2.867e-4, 3.19e-4, 3.371e-4,
01786     3.554e-4, 3.726e-4, 3.837e-4, 3.878e-4, 3.864e-4, 3.858e-4,
01787     3.841e-4, 3.852e-4, 3.815e-4, 3.762e-4, 3.618e-4, 3.579e-4,
01788     3.45e-4, 3.202e-4, 3.018e-4, 2.785e-4, 2.602e-4, 2.416e-4,
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5.038e-10, 5.128e-10, 5.143e-10, 5.071e-10, 5.019e-10, 5.025e-10,
5.183e-10, 5.496e-10, 5.877e-10, 6.235e-10, 6.42e-10, 6.234e-10,
5.698e-10, 4.916e-10, 4.022e-10, 3.126e-10, 2.282e-10, 1.639e-10,
1.142e-10, 7.919e-11, 5.69e-11, 4.313e-11, 3.413e-11, 2.807e-11,
2.41e-11, 2.166e-11, 2.024e-11, 1.946e-11, 1.929e-11, 1.963e-11,
2.035e-11, 2.162e-11, 2.305e-11, 2.493e-11, 2.748e-11, 3.048e-11,
3.413e-11, 3.754e-11, 4.155e-11, 4.635e-11, 5.11e-11, 5.734e-11,
6.338e-11, 6.99e-11, 7.611e-11, 8.125e-11, 8.654e-11, 8.951e-11,
9.182e-11, 9.31e-11, 9.273e-11, 9.094e-11, 8.849e-11, 8.662e-11,
8.67e-11, 8.972e-11, 9.566e-11, 1.025e-10, 1.083e-10, 1.111e-10,
1.074e-10, 9.771e-11, 8.468e-11, 6.958e-11, 5.47e-11, 4.04e-11,
2.94e-11, 2.075e-11, 1.442e-11, 1.01e-11, 7.281e-12, 5.409e-12,
4.138e-12, 3.304e-12, 2.784e-12, 2.473e-12, 2.273e-12, 2.186e-12,
2.118e-12, 2.066e-12, 1.958e-12, 1.818e-12, 1.675e-12, 1.509e-12,
1.349e-12, 1.171e-12, 9.838e-13, 8.213e-13, 6.765e-13, 5.378e-13,
4.161e-13, 3.119e-13, 2.279e-13, 1.637e-13, 1.152e-13, 8.112e-14,
5.919e-14, 4.47e-14, 3.492e-14, 2.811e-14, 2.319e-14, 1.948e-14,
1.66e-14, 1.432e-14, 1.251e-14, 1.109e-14, 1.006e-14, 9.45e-15,
9.384e-15, 1.012e-14, 1.216e-14, 1.636e-14, 2.305e-14, 3.488e-14,
5.572e-14, 8.479e-14, 1.265e-13, 1.905e-13, 2.73e-13, 3.809e-13,
4.955e-13, 6.303e-13, 7.861e-13, 9.427e-13, 1.097e-12, 1.212e-12,
1.328e-12, 1.415e-12, 1.463e-12, 1.495e-12, 1.571e-12, 1.731e-12,
1.981e-12, 2.387e-12, 2.93e-12, 3.642e-12, 4.584e-12, 5.822e-12,
7.278e-12, 9.193e-12, 1.135e-11, 1.382e-11, 1.662e-11, 1.958e-11,
2.286e-11, 2.559e-11, 2.805e-11, 2.988e-11, 3.106e-11, 3.182e-11,
3.2e-11, 3.258e-11, 3.362e-11, 3.558e-11, 3.688e-11, 3.8e-11,
3.929e-11, 4.062e-11, 4.186e-11, 4.293e-11, 4.48e-11, 4.643e-11,
4.704e-11, 4.571e-11, 4.206e-11, 3.715e-11, 3.131e-11, 2.541e-11,
1.978e-11, 1.508e-11, 1.146e-11, 8.7e-12, 6.603e-12, 5.162e-12,
4.157e-12, 3.408e-12, 2.829e-12, 2.405e-12, 2.071e-12, 1.826e-12,
1.648e-12, 1.542e-12, 1.489e-12, 1.485e-12, 1.493e-12, 1.545e-12,
1.637e-12, 1.814e-12, 2.061e-12, 2.312e-12, 2.651e-12, 3.03e-12,
3.46e-12, 3.901e-12, 4.306e-12, 4.721e-12, 5.008e-12, 5.281e-12,
5.541e-12, 5.791e-12, 6.115e-12, 6.442e-12, 6.68e-12, 6.791e-12,
6.831e-12, 6.839e-12, 6.946e-12, 7.128e-12, 7.537e-12, 8.036e-12,
8.392e-12, 8.526e-12, 8.11e-12, 7.325e-12, 6.329e-12, 5.183e-12,
4.081e-12, 2.985e-12, 2.141e-12, 1.492e-12, 1.015e-12, 6.684e-13,
4.414e-13, 2.987e-13, 2.038e-13, 1.391e-13, 9.86e-14, 7.24e-14,
5.493e-14, 4.288e-14, 3.427e-14, 2.787e-14, 2.296e-14, 1.909e-14,
1.598e-14, 1.344e-14, 1.135e-14, 9.616e-15, 8.169e-15, 6.957e-15,
5.938e-15, 5.08e-15, 4.353e-15, 3.738e-15, 3.217e-15, 2.773e-15,
2.397e-15, 2.077e-15, 1.805e-15, 1.575e-15, 1.382e-15, 1.221e-15,
1.09e-15, 9.855e-16, 9.068e-16, 8.537e-16, 8.27e-16, 8.29e-16,
8.634e-16, 9.359e-16, 1.055e-15, 1.233e-15, 1.486e-15, 1.839e-15,
2.326e-15, 2.998e-15, 3.934e-15, 5.256e-15, 7.164e-15, 9.984e-15,
1.427e-14, 2.099e-14, 3.196e-14, 5.121e-14, 7.908e-14, 1.131e-13,
1.602e-13, 2.239e-13, 3.075e-13, 4.134e-13, 5.749e-13, 7.886e-13,
1.071e-12, 1.464e-12, 2.032e-12, 2.8e-12, 3.732e-12, 4.996e-12,
6.483e-12, 8.143e-12, 1.006e-11, 1.238e-11, 1.484e-11, 1.744e-11,
2.02e-11, 2.274e-11, 2.562e-11, 2.848e-11, 3.191e-11, 3.617e-11,
4.081e-11, 4.577e-11, 4.937e-11, 5.204e-11, 5.401e-11, 5.462e-11,
5.507e-11, 5.51e-11, 5.605e-11, 5.686e-11, 5.739e-11, 5.766e-11,
5.74e-11, 5.754e-11, 5.761e-11, 5.777e-11, 5.712e-11, 5.51e-11,
5.088e-11, 4.438e-11, 3.728e-11, 2.994e-11, 2.305e-11, 1.715e-11,
1.256e-11, 9.208e-12, 6.745e-12, 5.014e-12, 3.785e-12, 2.9e-12,
2.239e-12, 1.757e-12, 1.414e-12, 1.142e-12, 9.482e-13, 8.01e-13,
6.961e-13, 6.253e-13, 5.735e-13, 5.433e-13, 5.352e-13, 5.493e-13,
5.706e-13, 6.068e-13, 6.531e-13, 7.109e-13, 7.767e-13, 8.59e-13,
9.792e-13, 1.142e-12, 1.371e-12, 1.65e-12, 1.957e-12, 2.302e-12,
2.705e-12, 3.145e-12, 3.608e-12, 4.071e-12, 4.602e-12, 5.133e-12,
5.572e-12, 5.987e-12, 6.248e-12, 6.533e-12, 6.757e-12, 6.935e-12,
7.224e-12, 7.422e-12, 7.538e-12, 7.547e-12, 7.495e-12, 7.543e-12,
7.725e-12, 8.139e-12, 8.627e-12, 9.146e-12, 9.443e-12, 9.318e-12,
8.649e-12, 7.512e-12, 6.261e-12, 4.915e-12, 3.647e-12, 2.597e-12,
1.785e-12, 1.242e-12, 8.66e-13, 6.207e-13, 4.61e-13, 3.444e-13,
2.634e-13, 2.1e-13, 1.725e-13, 1.455e-13, 1.237e-13, 1.085e-13,
9.513e-14, 7.978e-14, 6.603e-14, 5.288e-14, 4.084e-14, 2.952e-14,
2.157e-14, 1.593e-14, 1.199e-14, 9.267e-15, 7.365e-15, 6.004e-15,
4.995e-15, 4.218e-15, 3.601e-15, 3.101e-15, 2.692e-15, 2.36e-15,
2.094e-15, 1.891e-15, 1.755e-15, 1.699e-15, 1.755e-15, 1.987e-15,
2.506e-15, 3.506e-15, 5.289e-15, 8.311e-15, 1.325e-14, 2.129e-14,
3.237e-14, 4.595e-14, 6.441e-14, 8.433e-14, 1.074e-13, 1.383e-13,
1.762e-13, 2.281e-13, 2.831e-13, 3.523e-13, 4.38e-13, 5.304e-13,
6.29e-13, 7.142e-13, 8.032e-13, 8.934e-13, 9.888e-13, 1.109e-12,
1.261e-12, 1.462e-12, 1.74e-12, 2.099e-12, 2.535e-12, 3.008e-12,
3.462e-12, 3.856e-12, 4.098e-12, 4.239e-12, 4.234e-12, 4.132e-12,
3.986e-12, 3.866e-12, 3.829e-12, 3.742e-12, 3.705e-12, 3.694e-12,
3.765e-12, 3.849e-12, 3.929e-12, 4.056e-12, 4.092e-12, 4.047e-12,
3.792e-12, 3.407e-12, 2.953e-12, 2.429e-12, 1.931e-12, 1.46e-12,
1.099e-12, 8.199e-13, 6.077e-13, 4.449e-13, 3.359e-13, 2.524e-13,
1.881e-13, 1.391e-13, 1.02e-13, 7.544e-14, 5.555e-14, 4.22e-14,
3.321e-14, 2.686e-14, 2.212e-14, 1.78e-14, 1.369e-14, 1.094e-14,
9.13e-15, 8.101e-15, 7.828e-15, 8.393e-15, 1.012e-14, 1.259e-14,
1.538e-14, 1.961e-14, 2.619e-14, 3.679e-14, 5.049e-14, 6.917e-14,
8.88e-14, 1.115e-13, 1.373e-13, 1.619e-13, 1.878e-13, 2.111e-13,
2.33e-13, 2.503e-13, 2.613e-13, 2.743e-13, 2.826e-13, 2.976e-13,
3.162e-13, 3.36e-13, 3.491e-13, 3.541e-13, 3.595e-13, 3.608e-13,
```

```
    3.709e-13, 3.869e-13, 4.12e-13, 4.366e-13, 4.504e-13, 4.379e-13,
    3.955e-13, 3.385e-13, 2.741e-13, 2.089e-13, 1.427e-13, 9.294e-14,
    5.775e-14, 3.565e-14, 2.21e-14, 1.398e-14, 9.194e-15, 6.363e-15,
    4.644e-15, 3.55e-15, 2.808e-15, 2.274e-15, 1.871e-15, 1.557e-15,
    1.308e-15, 1.108e-15, 9.488e-16, 8.222e-16, 7.238e-16, 6.506e-16,
    6.008e-16, 5.742e-16, 5.724e-16, 5.991e-16, 6.625e-16, 7.775e-16,
    9.734e-16, 1.306e-15, 1.88e-15, 2.879e-15, 4.616e-15, 7.579e-15,
    1.248e-14, 2.03e-14, 3.244e-14, 5.171e-14, 7.394e-14, 9.676e-14,
    1.199e-13, 1.467e-13, 1.737e-13, 2.02e-13, 2.425e-13, 3.016e-13,
    3.7e-13, 4.617e-13, 5.949e-13, 7.473e-13, 9.378e-13, 1.191e-12,
    1.481e-12, 1.813e-12, 2.232e-12, 2.722e-12, 3.254e-12, 3.845e-12,
    4.458e-12, 5.048e-12, 5.511e-12, 5.898e-12, 6.204e-12, 6.293e-12,
    6.386e-12, 6.467e-12, 6.507e-12, 6.466e-12, 6.443e-12, 6.598e-12,
    6.873e-12, 7.3e-12, 7.816e-12, 8.368e-12, 8.643e-12, 8.466e-12,
    7.871e-12, 6.853e-12, 5.714e-12, 4.482e-12, 3.392e-12, 2.613e-12,
    2.008e-12, 1.562e-12, 1.228e-12, 9.888e-13, 7.646e-13, 5.769e-13,
    4.368e-13, 3.324e-13, 2.508e-13, 1.916e-13
  };

  static double xfcrev[15] =
    { 1.003, 1.009, 1.015, 1.023, 1.029, 1.033, 1.037,
    1.039, 1.04, 1.046, 1.036, 1.027, 1.01, 1.002, 1.
  };

  double sfac;

  /* Get H2O continuum absorption... */
  double xw = nu / 10 + 1;
  if (xw >= 1 && xw < 2001) {
    int iw = (int) xw;
    double dw = xw - iw;
    double ew = 1 - dw;
    double cw296 = ew * h2o296[iw - 1] + dw * h2o296[iw];
    double cw260 = ew * h2o260[iw - 1] + dw * h2o260[iw];
    double cwfrn = ew * h2ofrn[iw - 1] + dw * h2ofrn[iw];
    if (nu <= 820 || nu >= 960) {
      sfac = 1;
    } else {
      double xx = (nu - 820) / 10;
      int ix = (int) xx;
      double dx = xx - ix;
      sfac = (1 - dx) * xfcrev[ix] + dx * xfcrev[ix + 1];
    }
    double ctwslf =
      sfac * cw296 * pow(cw260 / cw296, (296 - t) / (296 - 260));
    double vf2 = POW2(nu - 370);
    double vf6 = POW3(vf2);
    double fscal = 36100 / (vf2 + vf6 * 1e-8 + 36100) * -.25 + 1;
    double ctwfrn = cwfrn * fscal;
    double a1 = nu * u * tanh(.7193876 / t * nu);
    double a2 = 296 / t;
    double a3 = p / P0 * (q * ctwslf + (1 - q) * ctwfrn) * 1e-20;
    return a1 * a2 * a3;
  } else
    return 0;
}
```

5.17.2.8 ctmn2()

```
double ctmn2 (
        double nu,
        double p,
        double t )
```

Compute nitrogen continuum (absorption coefficient).

Definition at line 2805 of file jurassic.c.

```
              {

  static double ba[98] = { 0., 4.45e-8, 5.22e-8, 6.46e-8, 7.75e-8, 9.03e-8,
    1.06e-7, 1.21e-7, 1.37e-7, 1.57e-7, 1.75e-7, 2.01e-7, 2.3e-7,
    2.59e-7, 2.95e-7, 3.26e-7, 3.66e-7, 4.05e-7, 4.47e-7, 4.92e-7,
    5.34e-7, 5.84e-7, 6.24e-7, 6.67e-7, 7.14e-7, 7.26e-7, 7.54e-7,
    7.84e-7, 8.09e-7, 8.42e-7, 8.62e-7, 8.87e-7, 9.11e-7, 9.36e-7,
    9.76e-7, 1.03e-6, 1.11e-6, 1.23e-6, 1.39e-6, 1.61e-6, 1.76e-6,
    1.94e-6, 1.97e-6, 1.87e-6, 1.75e-6, 1.56e-6, 1.42e-6, 1.35e-6,
    1.32e-6, 1.29e-6, 1.29e-6, 1.29e-6, 1.3e-6, 1.32e-6, 1.33e-6,
    1.34e-6, 1.35e-6, 1.33e-6, 1.31e-6, 1.29e-6, 1.24e-6, 1.2e-6,
    1.16e-6, 1.1e-6, 1.04e-6, 9.96e-7, 9.38e-7, 8.63e-7, 7.98e-7,
    7.26e-7, 6.55e-7, 5.94e-7, 5.35e-7, 4.74e-7, 4.24e-7, 3.77e-7,
```

```
    3.33e-7, 2.96e-7, 2.63e-7, 2.34e-7, 2.08e-7, 1.85e-7, 1.67e-7,
    1.47e-7, 1.32e-7, 1.2e-7, 1.09e-7, 9.85e-8, 9.08e-8, 8.18e-8,
    7.56e-8, 6.85e-8, 6.14e-8, 5.83e-8, 5.77e-8, 5e-8, 4.32e-8, 0.
  };

  static double betaa[98] = { 802., 802., 761., 722., 679., 646., 609., 562.,
    511., 472., 436., 406., 377., 355., 338., 319., 299., 278., 255.,
    233., 208., 184., 149., 107., 66., 25., -13., -49., -82., -104.,
    -119., -130., -139., -144., -146., -146., -147., -148., -150.,
    -153., -160., -169., -181., -189., -195., -200., -205., -209.,
    -211., -210., -210., -209., -205., -199., -190., -180., -168.,
    -157., -143., -126., -108., -89., -63., -32., 1., 35., 65., 95.,
    121., 141., 152., 161., 164., 164., 161., 155., 148., 143., 137.,
    133., 131., 133., 139., 150., 165., 187., 213., 248., 284., 321.,
    372., 449., 514., 569., 609., 642., 673., 673.
  };

  static double nua[98] = { 2120., 2125., 2130., 2135., 2140., 2145., 2150.,
    2155., 2160., 2165., 2170., 2175., 2180., 2185., 2190., 2195.,
    2200., 2205., 2210., 2215., 2220., 2225., 2230., 2235., 2240.,
    2245., 2250., 2255., 2260., 2265., 2270., 2275., 2280., 2285.,
    2290., 2295., 2300., 2305., 2310., 2315., 2320., 2325., 2330.,
    2335., 2340., 2345., 2350., 2355., 2360., 2365., 2370., 2375.,
    2380., 2385., 2390., 2395., 2400., 2405., 2410., 2415., 2420.,
    2425., 2430., 2435., 2440., 2445., 2450., 2455., 2460., 2465.,
    2470., 2475., 2480., 2485., 2490., 2495., 2500., 2505., 2510.,
    2515., 2520., 2525., 2530., 2535., 2540., 2545., 2550., 2555.,
    2560., 2565., 2570., 2575., 2580., 2585., 2590., 2595., 2600., 2605.
  };

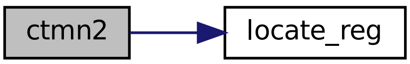
  const double q_n2 = 0.79, t0 = 273.0, tr = 296.0;

  /* Check wavenumber range... */
  if (nu < nua[0] || nu > nua[97])
    return 0;

  /* Interpolate B and beta... */
  int idx = locate_reg(nua, 98, nu);
  double b = LIN(nua[idx], ba[idx], nua[idx + 1], ba[idx + 1], nu);
  double beta = LIN(nua[idx], betaa[idx], nua[idx + 1], betaa[idx + 1], nu);

  /* Compute absorption coefficient... */
  return 0.1 * POW2(p / P0 * t0 / t) * exp(beta * (1 / tr - 1 / t))
    * q_n2 * b * (q_n2 + (1 - q_n2) * (1.294 - 0.4545 * t / tr));
}
```

Here is the call graph for this function:



5.17.2.9 ctmo2()

```
double ctmo2 (
        double nu,
        double p,
        double t )
```

Compute oxygen continuum (absorption coefficient).

Definition at line 2869 of file jurassic.c.

```
              {

  static double ba[90] = { 0., .061, .074, .084, .096, .12, .162, .208, .246,
    .285, .314, .38, .444, .5, .571, .673, .768, .853, .966, 1.097,
```

```
    1.214, 1.333, 1.466, 1.591, 1.693, 1.796, 1.922, 2.037, 2.154,
    2.264, 2.375, 2.508, 2.671, 2.847, 3.066, 3.417, 3.828, 4.204,
    4.453, 4.599, 4.528, 4.284, 3.955, 3.678, 3.477, 3.346, 3.29,
    3.251, 3.231, 3.226, 3.212, 3.192, 3.108, 3.033, 2.911, 2.798,
    2.646, 2.508, 2.322, 2.13, 1.928, 1.757, 1.588, 1.417, 1.253,
    1.109, .99, .888, .791, .678, .587, .524, .464, .403, .357, .32,
    .29, .267, .242, .215, .182, .16, .146, .128, .103, .087, .081,
    .071, .064, 0.
  };

  static double betaa[90] = { 467., 467., 400., 315., 379., 368., 475., 521.,
    531., 512., 442., 444., 430., 381., 335., 324., 296., 248., 215.,
    193., 158., 127., 101., 71., 31., -6., -26., -47., -63., -79.,
    -88., -88., -87., -90., -98., -99., -109., -134., -160., -167.,
    -164., -158., -153., -151., -156., -166., -168., -173., -170.,
    -161., -145., -126., -108., -84., -59., -29., 4., 41., 73., 97.,
    123., 159., 198., 220., 242., 256., 281., 311., 334., 319., 313.,
    321., 323., 310., 315., 320., 335., 361., 378., 373., 338., 319.,
    346., 322., 291., 290., 350., 371., 504., 504.
  };

  static double nua[90] = { 1360., 1365., 1370., 1375., 1380., 1385., 1390.,
    1395., 1400., 1405., 1410., 1415., 1420., 1425., 1430., 1435.,
    1440., 1445., 1450., 1455., 1460., 1465., 1470., 1475., 1480.,
    1485., 1490., 1495., 1500., 1505., 1510., 1515., 1520., 1525.,
    1530., 1535., 1540., 1545., 1550., 1555., 1560., 1565., 1570.,
    1575., 1580., 1585., 1590., 1595., 1600., 1605., 1610., 1615.,
    1620., 1625., 1630., 1635., 1640., 1645., 1650., 1655., 1660.,
    1665., 1670., 1675., 1680., 1685., 1690., 1695., 1700., 1705.,
    1710., 1715., 1720., 1725., 1730., 1735., 1740., 1745., 1750.,
    1755., 1760., 1765., 1770., 1775., 1780., 1785., 1790., 1795.,
    1800., 1805.
  };

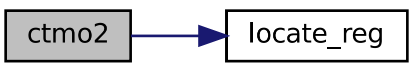
  const double q_o2 = 0.21, t0 = 273, tr = 296;

  /* Check wavenumber range... */
  if (nu < nua[0] || nu > nua[89])
    return 0;

  /* Interpolate B and beta... */
  int idx = locate_reg(nua, 90, nu);
  double b = LIN(nua[idx], ba[idx], nua[idx + 1], ba[idx + 1], nu);
  double beta = LIN(nua[idx], betaa[idx], nua[idx + 1], betaa[idx + 1], nu);

  /* Compute absorption coefficient... */
  return 0.1 * POW2(p / P0 * t0 / t) * exp(beta * (1 / tr - 1 / t)) * q_o2 *
    b;
}
```

Here is the call graph for this function:



5.17.2.10 copy_atm()

```
void copy_atm (
    ctl_t * ctl,
    atm_t * atm_dest,
    atm_t * atm_src,
    int init )
```

Copy and initialize atmospheric data.

Definition at line 2928 of file jurassic.c.

```
            {

  /* Data size... */
  size_t s = (size_t) atm_src->np * sizeof(double);

  /* Copy data... */
  atm_dest->np = atm_src->np;
  memcpy(atm_dest->time, atm_src->time, s);
  memcpy(atm_dest->z, atm_src->z, s);
  memcpy(atm_dest->lon, atm_src->lon, s);
  memcpy(atm_dest->lat, atm_src->lat, s);
  memcpy(atm_dest->p, atm_src->p, s);
  memcpy(atm_dest->t, atm_src->t, s);
  for (int ig = 0; ig < ctl->ng; ig++)
    memcpy(atm_dest->q[ig], atm_src->q[ig], s);
  for (int iw = 0; iw < ctl->nw; iw++)
    memcpy(atm_dest->k[iw], atm_src->k[iw], s);
  atm_dest->clz = atm_src->clz;
  atm_dest->cldz = atm_src->cldz;
  for (int icl = 0; icl < ctl->ncl; icl++)
    atm_dest->clk[icl] = atm_src->clk[icl];
  atm_dest->sfz = atm_src->sfz;
  atm_dest->sfp = atm_src->sfp;
  atm_dest->sft = atm_src->sft;
  for (int isf = 0; isf < ctl->nsf; isf++)
    atm_dest->sfeps[isf] = atm_src->sfeps[isf];

  /* Initialize... */
  if (init)
    for (int ip = 0; ip < atm_dest->np; ip++) {
      atm_dest->p[ip] = 0;
      atm_dest->t[ip] = 0;
      for (int ig = 0; ig < ctl->ng; ig++)
        atm_dest->q[ig][ip] = 0;
      for (int iw = 0; iw < ctl->nw; iw++)
        atm_dest->k[iw][ip] = 0;
      atm_dest->clz = 0;
      atm_dest->cldz = 0;
      for (int icl = 0; icl < ctl->ncl; icl++)
        atm_dest->clk[icl] = 0;
      atm_dest->sfz = 0;
      atm_dest->sfp = 0;
      atm_dest->sft = 0;
      for (int isf = 0; isf < ctl->nsf; isf++)
        atm_dest->sfeps[isf] = 1;
    }
}
```

5.17.2.11 copy_obs()

```
void copy_obs (
    ctl_t * ctl,
    obs_t * obs_dest,
    obs_t * obs_src,
    int init )
```

Copy and initialize observation data.

Definition at line 2982 of file jurassic.c.

```
            {

  /* Data size... */
  size_t s = (size_t) obs_src->nr * sizeof(double);

  /* Copy data... */
  obs_dest->nr = obs_src->nr;
  memcpy(obs_dest->time, obs_src->time, s);
  memcpy(obs_dest->obsz, obs_src->obsz, s);
  memcpy(obs_dest->obslon, obs_src->obslon, s);
  memcpy(obs_dest->obslat, obs_src->obslat, s);
  memcpy(obs_dest->vpz, obs_src->vpz, s);
  memcpy(obs_dest->vplon, obs_src->vplon, s);
  memcpy(obs_dest->vplat, obs_src->vplat, s);
  memcpy(obs_dest->tpz, obs_src->tpz, s);
  memcpy(obs_dest->tplon, obs_src->tplon, s);
  memcpy(obs_dest->tplat, obs_src->tplat, s);
  for (int id = 0; id < ctl->nd; id++)
    memcpy(obs_dest->rad[id], obs_src->rad[id], s);
```

```
03005   for (int id = 0; id < ctl->nd; id++)
03006     memcpy(obs_dest->tau[id], obs_src->tau[id], s);
03007 
03008   /* Initialize... */
03009   if (init)
03010     for (int id = 0; id < ctl->nd; id++)
03011       for (int ir = 0; ir < obs_dest->nr; ir++)
03012         if (gsl_finite(obs_dest->rad[id][ir])) {
03013           obs_dest->rad[id][ir] = 0;
03014           obs_dest->tau[id][ir] = 0;
03015         }
03016 }
```

5.17.2.12 find_emitter()

```
int find_emitter (
            ctl_t * ctl,
            const char * emitter )
```

Find index of an emitter.

Definition at line 3020 of file jurassic.c.

```
03022                         {
03023 
03024   for (int ig = 0; ig < ctl->ng; ig++)
03025     if (strcasecmp(ctl->emitter[ig], emitter) == 0)
03026       return ig;
03027 
03028   return -1;
03029 }
```

5.17.2.13 formod()

```
void formod (
            ctl_t * ctl,
            atm_t * atm,
            obs_t * obs )
```

Determine ray paths and compute radiative transfer.

Definition at line 3033 of file jurassic.c.

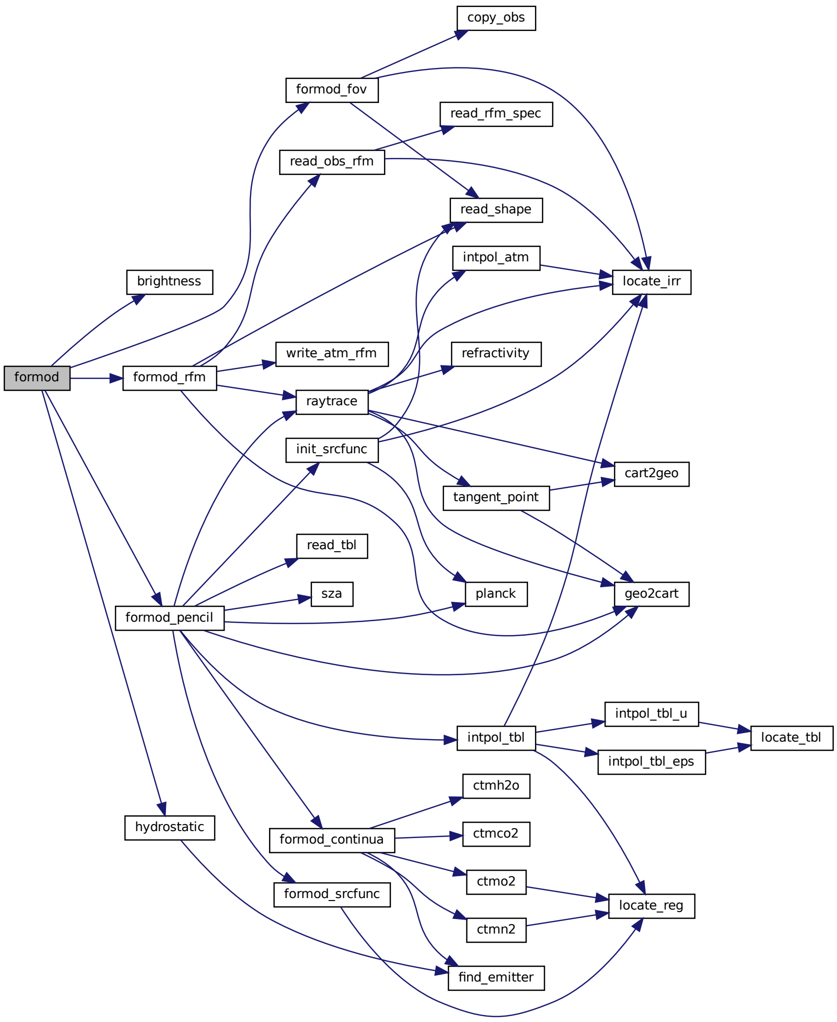
```
03036                 {
03037 
03038   int *mask;
03039 
03040   /* Allocate... */
03041   ALLOC(mask, int,
03042         ND * NR);
03043 
03044   /* Save observation mask... */
03045   for (int id = 0; id < ctl->nd; id++)
03046     for (int ir = 0; ir < obs->nr; ir++)
03047       mask[id * NR + ir] = !gsl_finite(obs->rad[id][ir]);
03048 
03049   /* Hydrostatic equilibrium... */
03050   hydrostatic(ctl, atm);
03051 
03052   /* EGA forward model... */
03053   if (ctl->formod == 1)
03054     for (int ir = 0; ir < obs->nr; ir++)
03055       formod_pencil(ctl, atm, obs, ir);
03056 
03057   /* Call RFM... */
03058   else if (ctl->formod == 2)
03059     formod_rfm(ctl, atm, obs);
03060 
03061   /* Apply field-of-view convolution... */
03062   formod_fov(ctl, obs);
03063 
03064   /* Convert radiance to brightness temperature... */
03065   if (ctl->write_bbt)
03066     for (int id = 0; id < ctl->nd; id++)
03067       for (int ir = 0; ir < obs->nr; ir++)
```

```
        obs->rad[id][ir] = brightness(obs->rad[id][ir], ctl->nu[id]);

    /* Apply observation mask... */
    for (int id = 0; id < ctl->nd; id++)
      for (int ir = 0; ir < obs->nr; ir++)
        if (mask[id * NR + ir])
          obs->rad[id][ir] = GSL_NAN;

    /* Free... */
    free(mask);
}
```

Here is the call graph for this function:



5.17.2.14 formod_continua() void formod_continua (

ctl_t * *ctl*,
los_t * *los*,
int *ip*,
double * *beta*)

Compute absorption coefficient of continua.

Definition at line 3082 of file jurassic.c.

```
                      {

  static int ig_co2 = -999, ig_h2o = -999;

  /* Extinction... */
  for (int id = 0; id < ctl->nd; id++)
    beta[id] = los->k[ip][id];

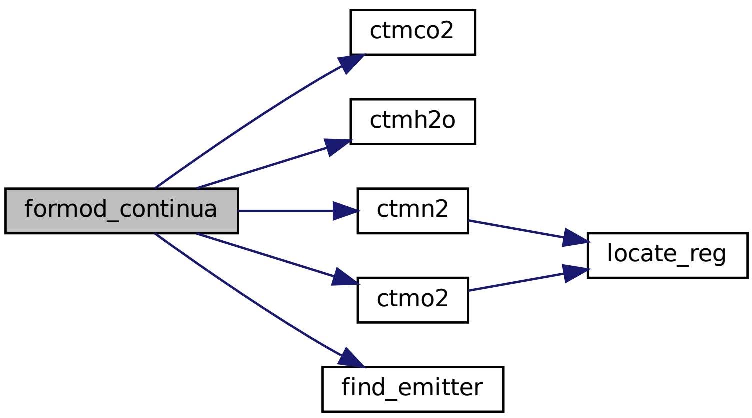
  /* CO2 continuum... */
  if (ctl->ctm_co2) {
    if (ig_co2 == -999)
      ig_co2 = find_emitter(ctl, "CO2");
    if (ig_co2 >= 0)
      for (int id = 0; id < ctl->nd; id++)
        beta[id] += ctmco2(ctl->nu[id], los->p[ip], los->t[ip],
                           los->u[ip][ig_co2]) / los->ds[ip];
  }

  /* H2O continuum... */
  if (ctl->ctm_h2o) {
    if (ig_h2o == -999)
      ig_h2o = find_emitter(ctl, "H2O");
    if (ig_h2o >= 0)
      for (int id = 0; id < ctl->nd; id++)
        beta[id] += ctmh2o(ctl->nu[id], los->p[ip], los->t[ip],
                           los->q[ip][ig_h2o], los->u[ip][ig_h2o])
          / los->ds[ip];
  }

  /* N2 continuum... */
  if (ctl->ctm_n2)
    for (int id = 0; id < ctl->nd; id++)
      beta[id] += ctmn2(ctl->nu[id], los->p[ip], los->t[ip]);

  /* O2 continuum... */
  if (ctl->ctm_o2)
    for (int id = 0; id < ctl->nd; id++)
      beta[id] += ctmo2(ctl->nu[id], los->p[ip], los->t[ip]);
}
```

Here is the call graph for this function:



5.17.2.15 formod_fov() void formod_fov (

ctl_t * *ctl*,

obs_t * *obs*)

Apply field of view convolution.

Definition at line 3128 of file jurassic.c.

```
                {

  static double dz[NSHAPE], w[NSHAPE];

  static int init = 0, n;

  obs_t *obs2;

  double rad[ND][NR], tau[ND][NR], z[NR];

  /* Do not take into account FOV... */
  if (ctl->fov[0] == '-')
    return;

  /* Initialize FOV data... */
  if (!init) {
    init = 1;
    read_shape(ctl->fov, dz, w, &n);
  }

  /* Allocate... */
  ALLOC(obs2, obs_t, 1);

  /* Copy observation data... */
  copy_obs(ctl, obs2, obs, 0);

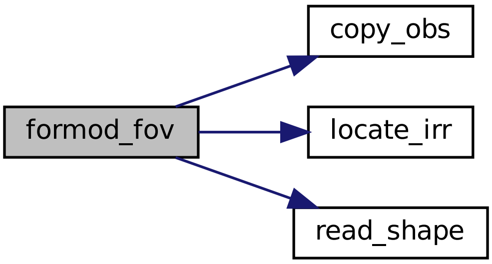
  /* Loop over ray paths... */
  for (int ir = 0; ir < obs->nr; ir++) {

    /* Get radiance and transmittance profiles... */
    int nz = 0;
    for (int ir2 = GSL_MAX(ir - NFOV, 0);
         ir2 < GSL_MIN(ir + 1 + NFOV, obs->nr); ir2++)
      if (obs->time[ir2] == obs->time[ir]) {
        z[nz] = obs2->vpz[ir2];
        for (int id = 0; id < ctl->nd; id++) {
          rad[id][nz] = obs2->rad[id][ir2];
          tau[id][nz] = obs2->tau[id][ir2];
        }
        nz++;
      }
    if (nz < 2)
      ERRMSG("Cannot apply FOV convolution!");

    /* Convolute profiles with FOV... */
    double wsum = 0;
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] = 0;
      obs->tau[id][ir] = 0;
    }
    for (int i = 0; i < n; i++) {
      double zfov = obs->vpz[ir] + dz[i];
      int idx = locate_irr(z, nz, zfov);
      for (int id = 0; id < ctl->nd; id++) {
        obs->rad[id][ir] += w[i]
          * LIN(z[idx], rad[id][idx], z[idx + 1], rad[id][idx + 1], zfov);
        obs->tau[id][ir] += w[i]
          * LIN(z[idx], tau[id][idx], z[idx + 1], tau[id][idx + 1], zfov);
      }
      wsum += w[i];
    }
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] /= wsum;
      obs->tau[id][ir] /= wsum;
    }
  }

  /* Free... */
  free(obs2);
}
```

Here is the call graph for this function:



5.17.2.16 formod_pencil()

```
void formod_pencil (
        ctl_t * ctl,
        atm_t * atm,
        obs_t * obs,
        int ir )
```

Compute radiative transfer for a pencil beam.

Definition at line 3203 of file jurassic.c.

```
           {

  static tbl_t *tbl;

  static int init = 0;

  los_t *los;

  double beta_ctm[ND], rad[ND], tau[ND], tau_refl[ND],
    tau_path[ND][NG], tau_gas[ND], x0[3], x1[3];

  /* Initialize look-up tables... */
  if (!init) {
    init = 1;
    ALLOC(tbl, tbl_t, 1);
    read_tbl(ctl, tbl);
    init_srcfunc(ctl, tbl);
  }

  /* Allocate... */
  ALLOC(los, los_t, 1);

  /* Initialize... */
  for (int id = 0; id < ctl->nd; id++) {
    rad[id] = 0;
    tau[id] = 1;
    for (int ig = 0; ig < ctl->ng; ig++)
      tau_path[id][ig] = 1;
  }

  /* Raytracing... */
  raytrace(ctl, atm, obs, los, ir);

  /* Loop over LOS points... */
  for (int ip = 0; ip < los->np; ip++) {

    /* Get trace gas transmittance... */
    intpol_tbl(ctl, tbl, los, ip, tau_path, tau_gas);

    /* Get continuum absorption... */
```

```
    formod_continua(ctl, los, ip, beta_ctm);

    /* Compute Planck function... */
    formod_srcfunc(ctl, tbl, los->t[ip], los->src[ip]);

    /* Loop over channels... */
    for (int id = 0; id < ctl->nd; id++)
      if (tau_gas[id] > 0) {

        /* Get segment emissivity... */
        los->eps[ip][id] = 1 - tau_gas[id] * exp(-beta_ctm[id] * los->ds[ip]);

        /* Compute radiance... */
        rad[id] += los->src[ip][id] * los->eps[ip][id] * tau[id];

        /* Compute path transmittance... */
        tau[id] *= (1 - los->eps[ip][id]);
      }
  }

  /* Check whether LOS hit the ground... */
  if (ctl->sftype >= 1 && los->sft > 0) {

    /* Add surface emissions... */
    double src_sf[ND];
    formod_srcfunc(ctl, tbl, los->sft, src_sf);
    for (int id = 0; id < ctl->nd; id++)
      rad[id] += los->sfeps[id] * src_sf[id] * tau[id];

    /* Check reflectivity... */
    int refl = 0;
    if (ctl->sftype >= 2)
      for (int id = 0; id < ctl->nd; id++)
        if (los->sfeps[id] < 1) {
          refl = 1;
          break;
        }

    /* Calculate reflection... */
    if (refl) {

      /* Initialize... */
      for (int id = 0; id < ctl->nd; id++)
        tau_refl[id] = 1;

      /* Add down-welling radiance... */
      for (int ip = los->np - 1; ip >= 0; ip--)
        for (int id = 0; id < ctl->nd; id++) {
          rad[id] += los->src[ip][id] * los->eps[ip][id] * tau_refl[id]
            * tau[id] * (1 - los->sfeps[id]);
          tau_refl[id] *= (1 - los->eps[ip][id]);
        }

      /* Add solar term... */
      if (ctl->sftype >= 3) {

        /* Get solar zenith angle... */
        double sza2;
        if (ctl->sfsza < 0)
          sza2 =
            sza(obs->time[ir], los->lon[los->np - 1], los->lat[los->np - 1]);
        else
          sza2 = ctl->sfsza;

        /* Check solar zenith angle... */
        if (sza2 < 89.999) {

          /* Get angle of incidence... */
          geo2cart(los->z[los->np - 1], los->lon[los->np - 1],
                   los->lat[los->np - 1], x0);
          geo2cart(los->z[0], los->lon[0], los->lat[0], x1);
          for (int i = 0; i < 3; i++)
            x1[i] -= x0[i];
          double cosa = DOTP(x0, x1) / NORM(x0) / NORM(x1);

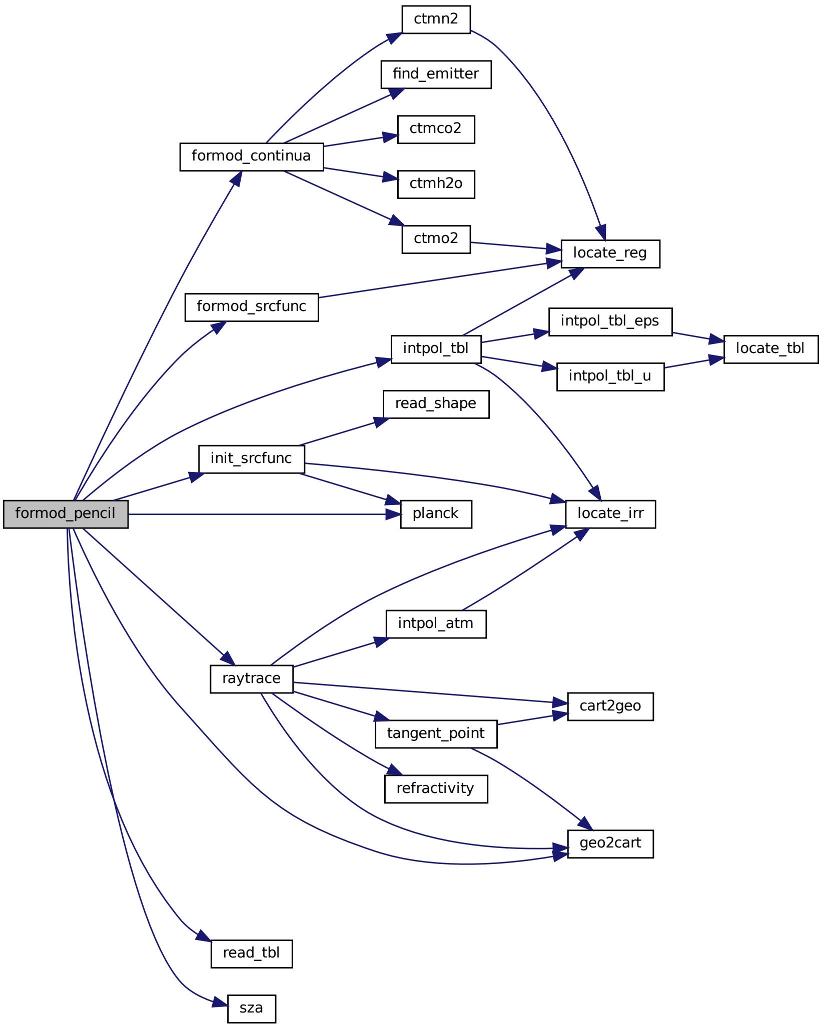
          /* Get ratio of SZA and incident radiation... */
          double rcos = cosa / cos(sza2 * M_PI / 180.);

          /* Add solar radiation... */
          for (int id = 0; id < ctl->nd; id++)
            rad[id] += 6.764e-5 / (2. * M_PI) * planck(TSUN, ctl->nu[id])
              * tau_refl[id] * (1 - los->sfeps[id]) * tau[id] * rcos;
        }
      }
    }
  }
```

```
  /* Copy results... */
  for (int id = 0; id < ctl->nd; id++) {
    obs->rad[id][ir] = rad[id];
    obs->tau[id][ir] = tau[id];
  }

  /* Free... */
  free(los);
}
```

Here is the call graph for this function:



5.17.2.17 formod_rfm()

```
void formod_rfm (
    ctl_t * ctl,
    atm_t * atm,
    obs_t * obs )
```

Apply RFM for radiative transfer calculations.

Definition at line 3346 of file jurassic.c.

```
                {

  los_t *los;

  FILE *out;

  char cmd[2 * LEN], filename[2 * LEN],
    rfmflg[LEN] = { "RAD TRA MIX LIN SFC" };

  double f[NSHAPE], nu[NSHAPE], nu0, nu1, obsz = -999, tsurf,
    xd[3], xo[3], xv[3], z[NR], zmin, zmax;

  int i, id, ig, ip, ir, iw, n, nadir = 0;

  /* Allocate... */
  ALLOC(los, los_t, 1);

  /* Check observer positions... */
  for (ir = 1; ir < obs->nr; ir++)
    if (obs->obsz[ir] != obs->obsz[0]
        || obs->obslon[ir] != obs->obslon[0]
        || obs->obslat[ir] != obs->obslat[0])
      ERRMSG("RFM interface requires identical observer positions!");

  /* Check extinction data... */
  for (iw = 0; iw < ctl->nw; iw++)
    for (ip = 0; ip < atm->np; ip++)
      if (atm->k[iw][ip] != 0)
        ERRMSG("RFM interface cannot handle extinction data!");

  /* Get altitude range of atmospheric data... */
  gsl_stats_minmax(&zmin, &zmax, atm->z, 1, (size_t) atm->np);

  /* Observer within atmosphere? */
  if (obs->obsz[0] >= zmin && obs->obsz[0] <= zmax) {
    obsz = obs->obsz[0];
    strcat(rfmflg, " OBS");
  }

  /* Determine tangent altitude or air mass factor... */
  for (ir = 0; ir < obs->nr; ir++) {

    /* Raytracing... */
    raytrace(ctl, atm, obs, los, ir);

    /* Nadir? */
    if (obs->tpz[ir] <= zmin) {
      geo2cart(obs->obsz[ir], obs->obslon[ir], obs->obslat[ir], xo);
      geo2cart(obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], xv);
      for (i = 0; i < 3; i++)
        xd[i] = xo[i] - xv[i];
      z[ir] = NORM(xo) * NORM(xd) / DOTP(xo, xd);
      nadir++;
    } else
      z[ir] = obs->tpz[ir];
  }
  if (nadir > 0 && nadir < obs->nr)
    ERRMSG("Limb and nadir not simultaneously possible!");

  /* Nadir? */
  if (nadir)
    strcat(rfmflg, " NAD");

  /* Get surface temperature... */
  tsurf = atm->t[gsl_stats_min_index(atm->z, 1, (size_t) atm->np)];

  /* Refraction? */
  if (!nadir && !ctl->refrac)
    strcat(rfmflg, " GEO");

  /* Continua? */
  if (ctl->ctm_co2 || ctl->ctm_h2o || ctl->ctm_n2 || ctl->ctm_o2)
    strcat(rfmflg, " CTM");

  /* Write atmospheric data file... */
  write_atm_rfm("rfm.atm", ctl, atm);

  /* Loop over channels... */
  for (id = 0; id < ctl->nd; id++) {

    /* Read filter function... */
    sprintf(filename, "%s_%.4f.filt", ctl->tblbase, ctl->nu[id]);
    read_shape(filename, nu, f, &n);

    /* Set spectral range... */
    nu0 = nu[0];
    nu1 = nu[n - 1];
```

```
    /* Create RFM driver file... */
    if (!(out = fopen("rfm.drv", "w")))
      ERRMSG("Cannot create file!");
    fprintf(out, "*HDR\nRFM call by JURASSIC.\n");
    fprintf(out, "*FLG\n%s\n", rfmflg);
    fprintf(out, "*SPC\n%.4f %.4f 0.0005\n", nu0, nu1);
    fprintf(out, "*GAS\n");
    for (ig = 0; ig < ctl->ng; ig++)
      fprintf(out, "%s\n", ctl->emitter[ig]);
    fprintf(out, "*ATM\nrfm.atm\n");
    fprintf(out, "*TAN\n");
    for (ir = 0; ir < obs->nr; ir++)
      fprintf(out, "%g\n", z[ir]);
    fprintf(out, "*SFC\n%g 1.0\n", tsurf);
    if (obsz >= 0)
      fprintf(out, "*OBS\n%g\n", obsz);
    fprintf(out, "*HIT\n%s\n", ctl->rfmhit);
    fprintf(out, "*XSC\n");
    for (ig = 0; ig < ctl->ng; ig++)
      if (ctl->rfmxsc[ig][0] != '-')
        fprintf(out, "%s\n", ctl->rfmxsc[ig]);
    fprintf(out, "*END\n");
    fclose(out);

    /* Remove temporary files... */
    if (system("rm -f rfm.runlog rad_*.asc tra_*.asc"))
      ERRMSG("Cannot remove temporary files!");

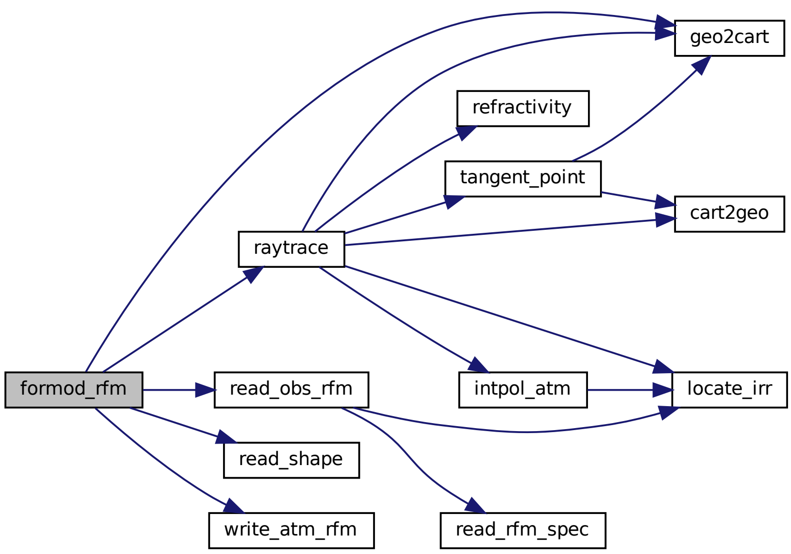
    /* Call RFM... */
    sprintf(cmd, "echo | %s", ctl->rfmbin);
    if (system(cmd))
      ERRMSG("Error while calling RFM!");

    /* Read data... */
    for (ir = 0; ir < obs->nr; ir++) {
      obs->rad[id][ir] = read_obs_rfm("rad", z[ir], nu, f, n) * 1e-5;
      obs->tau[id][ir] = read_obs_rfm("tra", z[ir], nu, f, n);
    }
  }

  /* Remove temporary files... */
  if (system("rm -f rfm.drv rfm.atm rfm.runlog rad_*.asc tra_*.asc"))
    ERRMSG("Error while removing temporary files!");

  /* Free... */
  free(los);
}
```

Here is the call graph for this function:



5.17.2.18 formod_srcfunc() void formod_srcfunc (

ctl_t * *ctl*,
tbl_t * *tbl*,
double *t*,
double * *src*)

Compute Planck source function.

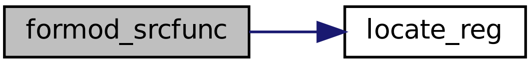
Definition at line 3487 of file jurassic.c.

```
                   {

  /* Determine index in temperature array... */
  int it = locate_reg(tbl->st, TBLNS, t);

  /* Interpolate Planck function value... */
  for (int id = 0; id < ctl->nd; id++)
    src[id] = LIN(tbl->st[it], tbl->sr[it][id],
                  tbl->st[it + 1], tbl->sr[it + 1][id], t);
}
```

Here is the call graph for this function:



5.17.2.19 geo2cart() void geo2cart (

double *z*,
double *lon*,
double *lat*,
double * *x*)

Convert geolocation to Cartesian coordinates.

Definition at line 3504 of file jurassic.c.

```
                 {

  double radius = z + RE;

  x[0] = radius * cos(lat / 180 * M_PI) * cos(lon / 180 * M_PI);
  x[1] = radius * cos(lat / 180 * M_PI) * sin(lon / 180 * M_PI);
  x[2] = radius * sin(lat / 180 * M_PI);
}
```

5.17.2.20 hydrostatic()

```
void hydrostatic (
    ctl_t * ctl,
    atm_t * atm )
```

Set hydrostatic equilibrium.

Definition at line 3519 of file jurassic.c.

```
                  {

  const double mmair = 28.96456e-3, mmh2o = 18.0153e-3;

  const int ipts = 20;

  static int ig_h2o = -999;

  double dzmin = 1e99, e = 0;

  int ipref = 0;

  /* Check reference height... */
  if (ctl->hydz < 0)
    return;

  /* Determine emitter index of H2O... */
  if (ig_h2o == -999)
    ig_h2o = find_emitter(ctl, "H2O");

  /* Find air parcel next to reference height... */
  for (int ip = 0; ip < atm->np; ip++)
    if (fabs(atm->z[ip] - ctl->hydz) < dzmin) {
      dzmin = fabs(atm->z[ip] - ctl->hydz);
      ipref = ip;
    }

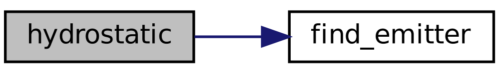
  /* Upper part of profile... */
  for (int ip = ipref + 1; ip < atm->np; ip++) {
    double mean = 0;
    for (int i = 0; i < ipts; i++) {
      if (ig_h2o >= 0)
        e = LIN(0.0, atm->q[ig_h2o][ip - 1],
                ipts - 1.0, atm->q[ig_h2o][ip], (double) i);
      mean += (e * mmh2o + (1 - e) * mmair)
        * G0 / RI
        / LIN(0.0, atm->t[ip - 1], ipts - 1.0, atm->t[ip], (double) i) / ipts;
    }

    /* Compute p(z,T)... */
    atm->p[ip] =
      exp(log(atm->p[ip - 1]) - mean * 1000 * (atm->z[ip] - atm->z[ip - 1]));
  }

  /* Lower part of profile... */
  for (int ip = ipref - 1; ip >= 0; ip--) {
    double mean = 0;
    for (int i = 0; i < ipts; i++) {
      if (ig_h2o >= 0)
        e = LIN(0.0, atm->q[ig_h2o][ip + 1],
                ipts - 1.0, atm->q[ig_h2o][ip], (double) i);
      mean += (e * mmh2o + (1 - e) * mmair)
        * G0 / RI
        / LIN(0.0, atm->t[ip + 1], ipts - 1.0, atm->t[ip], (double) i) / ipts;
    }

    /* Compute p(z,T)... */
    atm->p[ip] =
      exp(log(atm->p[ip + 1]) - mean * 1000 * (atm->z[ip] - atm->z[ip + 1]));
  }
}
```

Here is the call graph for this function:



5.17.2.21 idx2name()

```
void idx2name (
    ctl_t * ctl,
    int idx,
    char * quantity )
```

Determine name of state vector quantity for given index.

Definition at line 3585 of file jurassic.c.

```
                   {

  if (idx == IDXP)
    sprintf(quantity, "PRESSURE");

  if (idx == IDXT)
    sprintf(quantity, "TEMPERATURE");

  for (int ig = 0; ig < ctl->ng; ig++)
    if (idx == IDXQ(ig))
      sprintf(quantity, "%s", ctl->emitter[ig]);

  for (int iw = 0; iw < ctl->nw; iw++)
    if (idx == IDXK(iw))
      sprintf(quantity, "EXTINCT_WINDOW_%d", iw);

  if (idx == IDXCLZ)
    sprintf(quantity, "CLOUD_HEIGHT");

  if (idx == IDXCLDZ)
    sprintf(quantity, "CLOUD_DEPTH");

  for (int icl = 0; icl < ctl->ncl; icl++)
    if (idx == IDXCLK(icl))
      sprintf(quantity, "CLOUD_EXTINCT_%.4f", ctl->clnu[icl]);

  if (idx == IDXSFZ)
    sprintf(quantity, "SURFACE_HEIGHT");

  if (idx == IDXSFP)
    sprintf(quantity, "SURFACE_PRESSURE");

  if (idx == IDXSFT)
    sprintf(quantity, "SURFACE_TEMPERATURE");

  for (int isf = 0; isf < ctl->nsf; isf++)
    if (idx == IDXSFEPS(isf))
      sprintf(quantity, "SURFACE_EMISSIVITY_%.4f", ctl->sfnu[isf]);
}
```

5.17.2.22 init_srcfunc()

```
void init_srcfunc (
    ctl_t * ctl,
    tbl_t * tbl )
```

Initialize source function table.

Definition at line 3630 of file jurassic.c.

```
                {

  char filename[2 * LEN];

  double f[NSHAPE], nu[NSHAPE];

  int n;

  /* Write info... */
  LOG(1, "Initialize source function table...");

  /* Loop over channels... */
  for (int id = 0; id < ctl->nd; id++) {

    /* Read filter function... */
```

```
    sprintf(filename, "%s_%.4f.filt", ctl->tblbase, ctl->nu[id]);
    read_shape(filename, nu, f, &n);

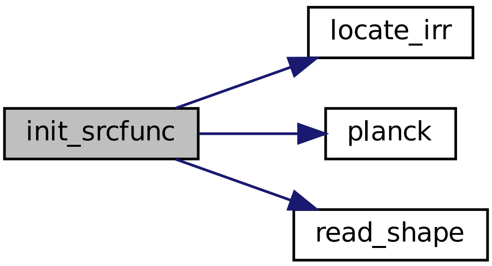
    /* Get minimum grid spacing... */
    double dnu = 1.0;
    for (int i = 1; i < n; i++)
      dnu = GSL_MIN(dnu, nu[i] - nu[i - 1]);

    /* Compute source function table... */
#pragma omp parallel for default(none) shared(ctl,tbl,id,nu,f,n,dnu)
    for (int it = 0; it < TBLNS; it++) {

      /* Set temperature... */
      tbl->st[it] = LIN(0.0, TMIN, TBLNS - 1.0, TMAX, (double) it);

      /* Integrate Planck function... */
      double fsum = tbl->sr[it][id] = 0;
      for (double fnu = nu[0]; fnu <= nu[n - 1]; fnu += dnu) {
        int i = locate_irr(nu, n, fnu);
        double ff = LIN(nu[i], f[i], nu[i + 1], f[i + 1], fnu);
        fsum += ff;
        tbl->sr[it][id] += ff * planck(tbl->st[it], fnu);
      }
      tbl->sr[it][id] /= fsum;
    }
  }
}
```

Here is the call graph for this function:



5.17.2.23 intpol_atm()

```
void intpol_atm (
    ctl_t * ctl,
    atm_t * atm,
    double z,
    double * p,
    double * t,
    double * q,
    double * k )
```

Interpolate atmospheric data.

Definition at line 3677 of file jurassic.c.

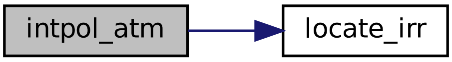
```
             {

  /* Get array index... */
  int ip = locate_irr(atm->z, atm->np, z);

  /* Interpolate... */
  *p = EXP(atm->z[ip], atm->p[ip], atm->z[ip + 1], atm->p[ip + 1], z);
```

```
  *t = LIN(atm->z[ip], atm->t[ip], atm->z[ip + 1], atm->t[ip + 1], z);
  for (int ig = 0; ig < ctl->ng; ig++)
    q[ig] =
      LIN(atm->z[ip], atm->q[ig][ip], atm->z[ip + 1], atm->q[ig][ip + 1], z);
  for (int iw = 0; iw < ctl->nw; iw++)
    k[iw] =
      LIN(atm->z[ip], atm->k[iw][ip], atm->z[ip + 1], atm->k[iw][ip + 1], z);
}
```

Here is the call graph for this function:



5.17.2.24 intpol_tbl()

```
void intpol_tbl (
        ctl_t * ctl,
        tbl_t * tbl,
        los_t * los,
        int ip,
        double tau_path[ND][NG],
        double tau_seg[ND] )
```

Get transmittance from look-up tables.

Definition at line 3702 of file jurassic.c.

```
                        {

  double eps, u;

  /* Loop over channels... */
  for (int id = 0; id < ctl->nd; id++) {

    /* Initialize... */
    tau_seg[id] = 1;

    /* Loop over emitters.... */
    for (int ig = 0; ig < ctl->ng; ig++) {

      /* Check size of table (pressure)... */
      if (tbl->np[id][ig] < 30)
        eps = 0;

      /* Check transmittance... */
      else if (tau_path[id][ig] < 1e-9)
        eps = 1;

      /* Interpolate... */
      else {

        /* Determine pressure and temperature indices... */
        int ipr = locate_irr(tbl->p[id][ig], tbl->np[id][ig], los->p[ip]);
        int it0 =
          locate_reg(tbl->t[id][ig][ipr], tbl->nt[id][ig][ipr], los->t[ip]);
        int it1 =
          locate_reg(tbl->t[id][ig][ipr + 1], tbl->nt[id][ig][ipr + 1],
                     los->t[ip]);

        /* Check size of table (temperature and column density)... */
        if (tbl->nt[id][ig][ipr] < 2 || tbl->nt[id][ig][ipr + 1] < 2
            || tbl->nu[id][ig][ipr][it0] < 2
            || tbl->nu[id][ig][ipr][it0 + 1] < 2
            || tbl->nu[id][ig][ipr + 1][it1] < 2
```

```
            || tbl->nu[id][ig][ipr + 1][it1 + 1] < 2)
          eps = 0;

        else {

          /* Get emissivities of extended path... */
          u = intpol_tbl_u(tbl, ig, id, ipr, it0, 1 - tau_path[id][ig]);
          double eps00
            = intpol_tbl_eps(tbl, ig, id, ipr, it0, u + los->u[ip][ig]);

          u = intpol_tbl_u(tbl, ig, id, ipr, it0 + 1, 1 - tau_path[id][ig]);
          double eps01 =
            intpol_tbl_eps(tbl, ig, id, ipr, it0 + 1, u + los->u[ip][ig]);

          u = intpol_tbl_u(tbl, ig, id, ipr + 1, it1, 1 - tau_path[id][ig]);
          double eps10 =
            intpol_tbl_eps(tbl, ig, id, ipr + 1, it1, u + los->u[ip][ig]);

          u =
            intpol_tbl_u(tbl, ig, id, ipr + 1, it1 + 1, 1 - tau_path[id][ig]);
          double eps11 =
            intpol_tbl_eps(tbl, ig, id, ipr + 1, it1 + 1, u + los->u[ip][ig]);

          /* Interpolate with respect to temperature... */
          eps00 = LIN(tbl->t[id][ig][ipr][it0], eps00,
                      tbl->t[id][ig][ipr][it0 + 1], eps01, los->t[ip]);
          eps11 = LIN(tbl->t[id][ig][ipr + 1][it1], eps10,
                      tbl->t[id][ig][ipr + 1][it1 + 1], eps11, los->t[ip]);

          /* Interpolate with respect to pressure... */
          eps00 = LIN(tbl->p[id][ig][ipr], eps00,
                      tbl->p[id][ig][ipr + 1], eps11, los->p[ip]);

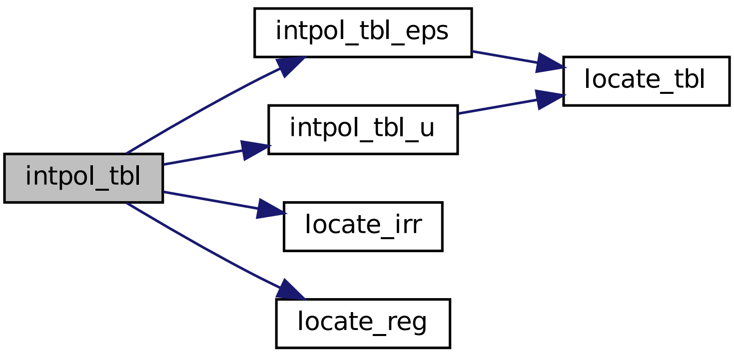
          /* Check emssivity range... */
          eps00 = GSL_MAX(GSL_MIN(eps00, 1), 0);

          /* Determine segment emissivity... */
          eps = 1 - (1 - eps00) / tau_path[id][ig];
        }
      }

      /* Get transmittance of extended path... */
      tau_path[id][ig] *= (1 - eps);

      /* Get segment transmittance... */
      tau_seg[id] *= (1 - eps);
    }
  }
}
```

Here is the call graph for this function:



5.17.2.25 intpol_tbl_eps()

```
double intpol_tbl_eps (
            tbl_t * tbl,
            int ig,
            int id,
            int ip,
            int it,
            double u )
```

Interpolate emissivity from look-up tables.

Definition at line 3797 of file jurassic.c.

```
                 {

  /* Lower boundary... */
  if (u < tbl->u[id][ig][ip][it][0])
    return LIN(0, 0, tbl->u[id][ig][ip][it][0], tbl->eps[id][ig][ip][it][0],
               u);

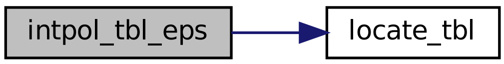
  /* Upper boundary... */
  else if (u > tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1])
    return LIN(tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               1e30, 1, u);

  /* Interpolation... */
  else {

    /* Get index... */
    int idx = locate_tbl(tbl->u[id][ig][ip][it], tbl->nu[id][ig][ip][it], u);

    /* Interpolate... */
    return
      LIN(tbl->u[id][ig][ip][it][idx], tbl->eps[id][ig][ip][it][idx],
          tbl->u[id][ig][ip][it][idx + 1], tbl->eps[id][ig][ip][it][idx + 1],
          u);
  }
}
```

Here is the call graph for this function:



5.17.2.26 intpol_tbl_u()

```
double intpol_tbl_u (
            tbl_t * tbl,
            int ig,
            int id,
            int ip,
            int it,
            double eps )
```

Interpolate column density from look-up tables.

Definition at line 3832 of file jurassic.c.

```
                   {

  /* Lower boundary... */
```

```
  if (eps < tbl->eps[id][ig][ip][it][0])
    return LIN(0, 0, tbl->eps[id][ig][ip][it][0], tbl->u[id][ig][ip][it][0],
               eps);

  /* Upper boundary... */
  else if (eps > tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1])
    return LIN(tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               1, 1e30, eps);

  /* Interpolation... */
  else {

    /* Get index... */
    int idx
      = locate_tbl(tbl->eps[id][ig][ip][it], tbl->nu[id][ig][ip][it], eps);

    /* Interpolate... */
    return
      LIN(tbl->eps[id][ig][ip][it][idx], tbl->u[id][ig][ip][it][idx],
          tbl->eps[id][ig][ip][it][idx + 1], tbl->u[id][ig][ip][it][idx + 1],
          eps);
  }
}
```

Here is the call graph for this function:

5.17.2.27 jsec2time()

```
void jsec2time (
        double jsec,
        int * year,
        int * mon,
        int * day,
        int * hour,
        int * min,
        int * sec,
        double * remain )
```

Convert seconds to date.

Definition at line 3868 of file jurassic.c.

```
                         {

  struct tm t0, *t1;

  t0.tm_year = 100;
  t0.tm_mon = 0;
  t0.tm_mday = 1;
  t0.tm_hour = 0;
  t0.tm_min = 0;
  t0.tm_sec = 0;

  time_t jsec0 = (time_t) jsec + timegm(&t0);
  t1 = gmtime(&jsec0);

  *year = t1->tm_year + 1900;
  *mon = t1->tm_mon + 1;
  *day = t1->tm_mday;
  *hour = t1->tm_hour;
```

```
  *min = t1->tm_min;
  *sec = t1->tm_sec;
  *remain = jsec - floor(jsec);
}
```

5.17.2.28 kernel()

```
void kernel (
    ctl_t * ctl,
    atm_t * atm,
    obs_t * obs,
    gsl_matrix * k )
```

Compute Jacobians.

Definition at line 3901 of file jurassic.c.

```
                         {

  atm_t *atm1;
  obs_t *obs1;

  gsl_vector *x0, *x1, *yy0, *yy1;

  int *iqa;

  /* Get sizes... */
  size_t m = k->size1;
  size_t n = k->size2;

  /* Allocate... */
  x0 = gsl_vector_alloc(n);
  yy0 = gsl_vector_alloc(m);
  ALLOC(iqa, int,
        N);

  /* Compute radiance for undisturbed atmospheric data... */
  formod(ctl, atm, obs);

  /* Compose vectors... */
  atm2x(ctl, atm, x0, iqa, NULL);
  obs2y(ctl, obs, yy0, NULL, NULL);

  /* Initialize kernel matrix... */
  gsl_matrix_set_zero(k);

  /* Loop over state vector elements... */
#pragma omp parallel for default(none) shared(ctl,atm,obs,k,x0,yy0,n,m,iqa) private(x1, yy1, atm1, obs1)
  for (size_t j = 0; j < n; j++) {

    /* Allocate... */
    x1 = gsl_vector_alloc(n);
    yy1 = gsl_vector_alloc(m);
    ALLOC(atm1, atm_t, 1);
    ALLOC(obs1, obs_t, 1);

    /* Set perturbation size... */
    double h;
    if (iqa[j] == IDXP)
      h = GSL_MAX(fabs(0.01 * gsl_vector_get(x0, j)), 1e-7);
    else if (iqa[j] == IDXT)
      h = 1.0;
    else if (iqa[j] >= IDXQ(0) && iqa[j] < IDXQ(ctl->ng))
      h = GSL_MAX(fabs(0.01 * gsl_vector_get(x0, j)), 1e-15);
    else if (iqa[j] >= IDXK(0) && iqa[j] < IDXK(ctl->nw))
      h = 1e-4;
    else if (iqa[j] == IDXCLZ || iqa[j] == IDXCLDZ)
      h = 1.0;
    else if (iqa[j] >= IDXCLK(0) && iqa[j] < IDXCLK(ctl->ncl))
      h = 1e-4;
    else if (iqa[j] == IDXSFZ)
      h = 0.1;
    else if (iqa[j] == IDXSFP)
      h = 10.0;
    else if (iqa[j] == IDXSFT)
      h = 1.0;
    else if (iqa[j] >= IDXSFEPS(0) && iqa[j] < IDXSFEPS(ctl->nsf))
      h = 1e-2;
    else
```

```
      ERRMSG("Cannot set perturbation size!");

    /* Disturb state vector element... */
    gsl_vector_memcpy(x1, x0);
    gsl_vector_set(x1, j, gsl_vector_get(x1, j) + h);
    copy_atm(ctl, atm1, atm, 0);
    copy_obs(ctl, obs1, obs, 0);
    x2atm(ctl, x1, atm1);

    /* Compute radiance for disturbed atmospheric data... */
    formod(ctl, atm1, obs1);

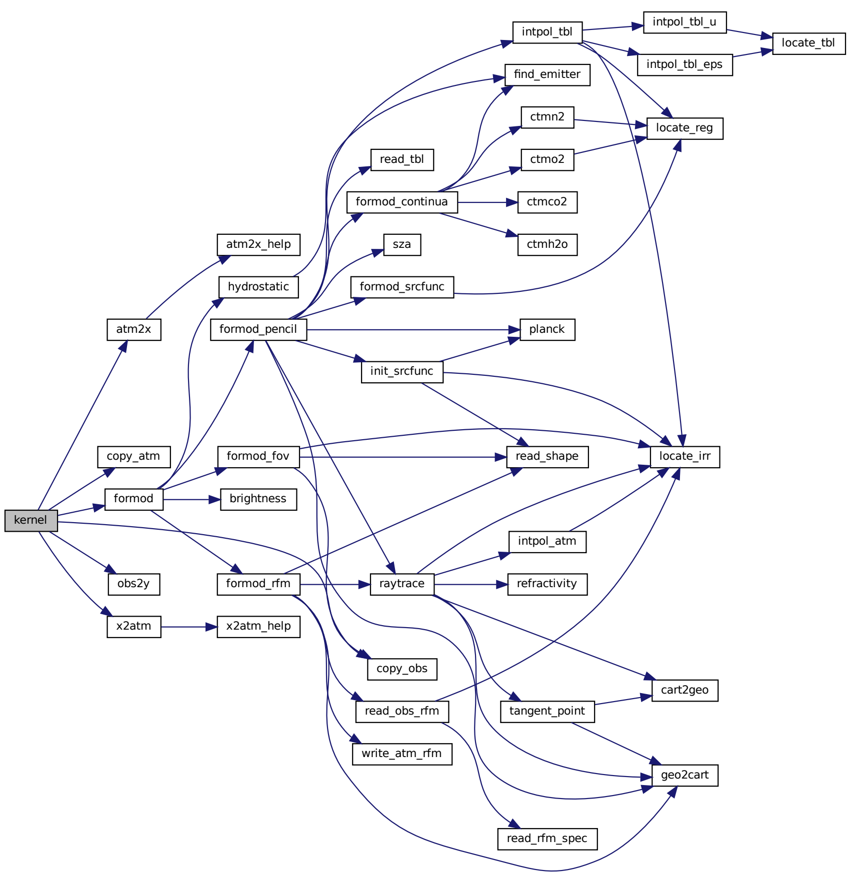
    /* Compose measurement vector for disturbed radiance data... */
    obs2y(ctl, obs1, yy1, NULL, NULL);

    /* Compute derivatives... */
    for (size_t i = 0; i < m; i++)
      gsl_matrix_set(k, i, j,
                     (gsl_vector_get(yy1, i) - gsl_vector_get(yy0, i)) / h);

    /* Free... */
    gsl_vector_free(x1);
    gsl_vector_free(yy1);
    free(atm1);
    free(obs1);
  }

  /* Free... */
  gsl_vector_free(x0);
  gsl_vector_free(yy0);
  free(iqa);
}
```

Here is the call graph for this function:



5.17.2.29 locate_irr()

```
int locate_irr (
    double * xx,
    int n,
    double x )
```

Find array index for irregular grid.

Definition at line 4002 of file jurassic.c.

```
                {

  int ilo = 0;
  int ihi = n - 1;
  int i = (ihi + ilo) » 1;

  if (xx[i] < xx[i + 1])
    while (ihi > ilo + 1) {
      i = (ihi + ilo) » 1;
      if (xx[i] > x)
        ihi = i;
      else
        ilo = i;
  } else
    while (ihi > ilo + 1) {
      i = (ihi + ilo) » 1;
      if (xx[i] <= x)
        ihi = i;
      else
        ilo = i;
    }

  return ilo;
}
```

5.17.2.30 locate_reg()

```
int locate_reg (
    double * xx,
    int n,
    double x )
```

Find array index for regular grid.

Definition at line 4032 of file jurassic.c.

```
                {

  /* Calculate index... */
  int i = (int) ((x - xx[0]) / (xx[1] - xx[0]));

  /* Check range... */
  if (i < 0)
    return 0;
  else if (i > n - 2)
    return n - 2;
  else
    return i;
}
```

5.17.2.31 locate_tbl()

```
int locate_tbl (
    float * xx,
    int n,
    double x )
```

Find array index in float array.

Definition at line 4051 of file jurassic.c.

```
                {

  int ilo = 0;
```

```
  int ihi = n - 1;
  int i = (ihi + ilo) » 1;

  while (ihi > ilo + 1) {
    i = (ihi + ilo) » 1;
    if (xx[i] > x)
      ihi = i;
    else
      ilo = i;
  }

  return ilo;
}
```

5.17.2.32 obs2y()

```
size_t obs2y (
    ctl_t * ctl,
    obs_t * obs,
    gsl_vector * y,
    int * ida,
    int * ira )
```

Compose measurement vector.

Definition at line 4073 of file jurassic.c.

```
                {

  size_t m = 0;

  /* Determine measurement vector... */
  for (int ir = 0; ir < obs->nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      if (gsl_finite(obs->rad[id][ir])) {
        if (y != NULL)
          gsl_vector_set(y, m, obs->rad[id][ir]);
        if (ida != NULL)
          ida[m] = id;
        if (ira != NULL)
          ira[m] = ir;
        m++;
      }

  return m;
}
```

5.17.2.33 planck()

```
double planck (
    double t,
    double nu )
```

Compute Planck function.

Definition at line 4100 of file jurassic.c.

```
                 {

  return C1 * POW3(nu) / gsl_expm1(C2 * nu / t);
}
```

5.17.2.34 raytrace() void raytrace (

```
ctl_t * ctl,
atm_t * atm,
obs_t * obs,
los_t * los,
int ir )
```

Do ray-tracing to determine LOS.

Definition at line 4109 of file jurassic.c.

```
                {

  const double h = 0.02, zrefrac = 60;

  double ds, ex0[3], ex1[3], k[NW], lat, lon, n, ng[3], norm,
    p, q[NG], t, x[3], xh[3], xobs[3], xvp[3], z = 1e99, zmax, zmin;

  int stop = 0;

  /* Initialize... */
  los->np = 0;
  los->sft = -999;
  obs->tpz[ir] = obs->vpz[ir];
  obs->tplon[ir] = obs->vplon[ir];
  obs->tplat[ir] = obs->vplat[ir];

  /* Get altitude range of atmospheric data... */
  gsl_stats_minmax(&zmin, &zmax, atm->z, 1, (size_t) atm->np);
  if (ctl->nsf > 0) {
    zmin = GSL_MAX(atm->sfz, zmin);
    if (atm->sfp > 0) {
      int ip = locate_irr(atm->p, atm->np, atm->sfp);
      double zip = LIN(log(atm->p[ip]), atm->z[ip],
                       log(atm->p[ip + 1]), atm->z[ip + 1], log(atm->sfp));
      zmin = GSL_MAX(zip, zmin);
    }
  }

  /* Check observer altitude... */
  if (obs->obsz[ir] < zmin)
    ERRMSG("Observer below surface!");

  /* Check view point altitude... */
  if (obs->vpz[ir] > zmax)
    return;

  /* Determine Cartesian coordinates for observer and view point... */
  geo2cart(obs->obsz[ir], obs->obslon[ir], obs->obslat[ir], xobs);
  geo2cart(obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], xvp);

  /* Determine initial tangent vector... */
  for (int i = 0; i < 3; i++)
    ex0[i] = xvp[i] - xobs[i];
  norm = NORM(ex0);
  for (int i = 0; i < 3; i++)
    ex0[i] /= norm;

  /* Observer within atmosphere... */
  for (int i = 0; i < 3; i++)
    x[i] = xobs[i];

  /* Observer above atmosphere (search entry point)... */
  if (obs->obsz[ir] > zmax) {
    double dmax = norm, dmin = 0;
    while (fabs(dmin - dmax) > 0.001) {
      double d = (dmax + dmin) / 2;
      for (int i = 0; i < 3; i++)
        x[i] = xobs[i] + d * ex0[i];
      cart2geo(x, &z, &lon, &lat);
      if (z <= zmax && z > zmax - 0.001)
        break;
      if (z < zmax - 0.0005)
        dmax = d;
      else
        dmin = d;
    }
  }

  /* Ray-tracing... */
  while (1) {

    /* Set step length... */
    ds = ctl->rayds;
```

```
    if (ctl->raydz > 0) {
      norm = NORM(x);
      for (int i = 0; i < 3; i++)
        xh[i] = x[i] / norm;
      double cosa = fabs(DOTP(ex0, xh));
      if (cosa != 0)
        ds = GSL_MIN(ctl->rayds, ctl->raydz / cosa);
    }

    /* Determine geolocation... */
    cart2geo(x, &z, &lon, &lat);

    /* Check if LOS hits the ground or has left atmosphere... */
    if (z < zmin || z > zmax) {
      stop = (z < zmin ? 2 : 1);
      double frac =
        ((z <
          zmin ? zmin : zmax) - los->z[los->np - 1]) / (z - los->z[los->np -
                                                                1]);
      geo2cart(los->z[los->np - 1], los->lon[los->np - 1],
               los->lat[los->np - 1], xh);
      for (int i = 0; i < 3; i++)
        x[i] = xh[i] + frac * (x[i] - xh[i]);
      cart2geo(x, &z, &lon, &lat);
      los->ds[los->np - 1] = ds * frac;
      ds = 0;
    }

    /* Interpolate atmospheric data... */
    intpol_atm(ctl, atm, z, &p, &t, q, k);

    /* Save data... */
    los->lon[los->np] = lon;
    los->lat[los->np] = lat;
    los->z[los->np] = z;
    los->p[los->np] = p;
    los->t[los->np] = t;
    for (int ig = 0; ig < ctl->ng; ig++)
      los->q[los->np][ig] = q[ig];
    for (int id = 0; id < ctl->nd; id++)
      los->k[los->np][id] = k[ctl->window[id]];
    los->ds[los->np] = ds;

    /* Add cloud extinction... */
    if (ctl->ncl > 0 && atm->cldz > 0) {
      double aux = exp(-0.5 * POW2((z - atm->clz) / atm->cldz));
      for (int id = 0; id < ctl->nd; id++) {
        int icl = locate_irr(ctl->clnu, ctl->ncl, ctl->nu[id]);
        los->k[los->np][id]
          += aux * LIN(ctl->clnu[icl], atm->clk[icl],
                       ctl->clnu[icl + 1], atm->clk[icl + 1], ctl->nu[id]);
      }
    }

    /* Increment and check number of LOS points... */
    if ((++los->np) > NLOS)
      ERRMSG("Too many LOS points!");

    /* Check stop flag... */
    if (stop) {

      /* Set surface temperature... */
      if (ctl->nsf > 0 && atm->sft > 0)
        t = atm->sft;
      los->sft = (stop == 2 ? t : -999);

      /* Set surface emissivity... */
      for (int id = 0; id < ctl->nd; id++) {
        los->sfeps[id] = 1.0;
        if (ctl->nsf > 0) {
          int isf = locate_irr(ctl->sfnu, ctl->nsf, ctl->nu[id]);
          los->sfeps[id] = LIN(ctl->sfnu[isf], atm->sfeps[isf],
                               ctl->sfnu[isf + 1], atm->sfeps[isf + 1],
                               ctl->nu[id]);
        }
      }

      /* Leave raytracer... */
      break;
    }

    /* Determine refractivity... */
    if (ctl->refrac && z <= zrefrac)
      n = 1 + refractivity(p, t);
    else
      n = 1;

```

```
    /* Construct new tangent vector (first term)... */
    for (int i = 0; i < 3; i++)
      ex1[i] = ex0[i] * n;

    /* Compute gradient of refractivity... */
    if (ctl->refrac && z <= zrefrac) {
      for (int i = 0; i < 3; i++)
        xh[i] = x[i] + 0.5 * ds * ex0[i];
      cart2geo(xh, &z, &lon, &lat);
      intpol_atm(ctl, atm, z, &p, &t, q, k);
      n = refractivity(p, t);
      for (int i = 0; i < 3; i++) {
        xh[i] += h;
        cart2geo(xh, &z, &lon, &lat);
        intpol_atm(ctl, atm, z, &p, &t, q, k);
        ng[i] = (refractivity(p, t) - n) / h;
        xh[i] -= h;
      }
    } else
      for (int i = 0; i < 3; i++)
        ng[i] = 0;

    /* Construct new tangent vector (second term)... */
    for (int i = 0; i < 3; i++)
      ex1[i] += ds * ng[i];

    /* Normalize new tangent vector... */
    norm = NORM(ex1);
    for (int i = 0; i < 3; i++)
      ex1[i] /= norm;

    /* Determine next point of LOS... */
    for (int i = 0; i < 3; i++)
      x[i] += 0.5 * ds * (ex0[i] + ex1[i]);

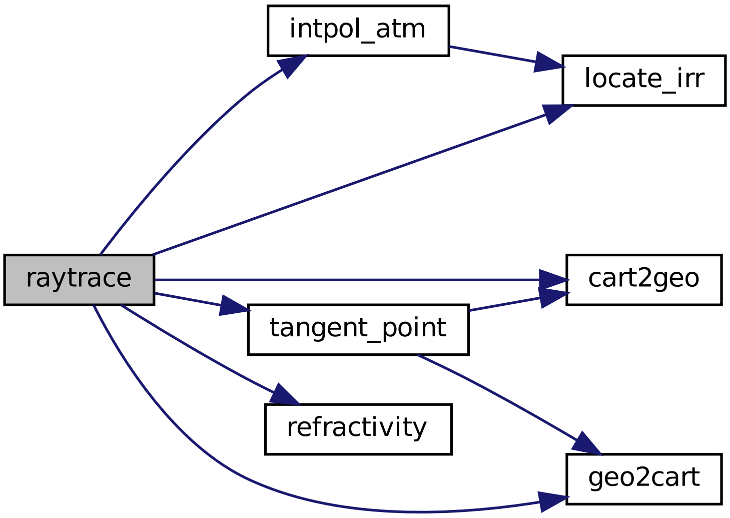
    /* Copy tangent vector... */
    for (int i = 0; i < 3; i++)
      ex0[i] = ex1[i];
  }

  /* Get tangent point (to be done before changing segment lengths!)... */
  tangent_point(los, &obs->tpz[ir], &obs->tplon[ir], &obs->tplat[ir]);

  /* Change segment lengths according to trapezoid rule... */
  for (int ip = los->np - 1; ip >= 1; ip--)
    los->ds[ip] = 0.5 * (los->ds[ip - 1] + los->ds[ip]);
  los->ds[0] *= 0.5;

  /* Compute column density... */
  for (int ip = 0; ip < los->np; ip++)
    for (int ig = 0; ig < ctl->ng; ig++)
      los->u[ip][ig] = 10 * los->q[ip][ig] * los->p[ip]
        / (KB * los->t[ip]) * los->ds[ip];
}
```

Here is the call graph for this function:



5.17.2.35 read_atm()

```
void read_atm (
    const char * dirname,
    const char * filename,
    ctl_t * ctl,
    atm_t * atm )
```

Read atmospheric data.

Definition at line 4331 of file jurassic.c.

```
04335                 {
04336 
04337   FILE *in;
04338 
04339   char file[LEN], line[LEN], *tok;
04340 
04341   /* Init... */
04342   atm->np = 0;
04343 
04344   /* Set filename... */
04345   if (dirname != NULL)
04346     sprintf(file, "%s/%s", dirname, filename);
04347   else
04348     sprintf(file, "%s", filename);
04349 
04350   /* Write info... */
04351   LOG(1, "Read atmospheric data: %s", file);
04352 
04353   /* Open file... */
04354   if (!(in = fopen(file, "r")))
04355     ERRMSG("Cannot open file!");
04356 
04357   /* Read line... */
04358   while (fgets(line, LEN, in)) {
04359 
04360     /* Read data... */
04361     TOK(line, tok, "%lg", atm->time[atm->np]);
04362     TOK(NULL, tok, "%lg", atm->z[atm->np]);
```

```
    TOK(NULL, tok, "%lg", atm->lon[atm->np]);
    TOK(NULL, tok, "%lg", atm->lat[atm->np]);
    TOK(NULL, tok, "%lg", atm->p[atm->np]);
    TOK(NULL, tok, "%lg", atm->t[atm->np]);
    for (int ig = 0; ig < ctl->ng; ig++)
      TOK(NULL, tok, "%lg", atm->q[ig][atm->np]);
    for (int iw = 0; iw < ctl->nw; iw++)
      TOK(NULL, tok, "%lg", atm->k[iw][atm->np]);
    if (ctl->ncl > 0 && atm->np == 0) {
      TOK(NULL, tok, "%lg", atm->clz);
      TOK(NULL, tok, "%lg", atm->cldz);
      for (int icl = 0; icl < ctl->ncl; icl++)
        TOK(NULL, tok, "%lg", atm->clk[icl]);
    }
    if (ctl->nsf > 0 && atm->np == 0) {
      TOK(NULL, tok, "%lg", atm->sfz);
      TOK(NULL, tok, "%lg", atm->sfp);
      TOK(NULL, tok, "%lg", atm->sft);
      for (int isf = 0; isf < ctl->nsf; isf++)
        TOK(NULL, tok, "%lg", atm->sfeps[isf]);
    }

    /* Increment data point counter... */
    if ((++atm->np) > NP)
      ERRMSG("Too many data points!");
  }

  /* Close file... */
  fclose(in);

  /* Check number of points... */
  if (atm->np < 1)
    ERRMSG("Could not read any data!");
}
```

5.17.2.36 read_ctl()

```
void read_ctl (
    int argc,
    char * argv[],
    ctl_t * ctl )
```

Read forward model control parameters.

Definition at line 4400 of file jurassic.c.

```
                {

  /* Write info... */
  LOG(1, "\nJuelich Rapid Spectral Simulation Code (JURASSIC)\n"
      "(executable: %s | version: %s | compiled: %s, %s)\n",
      argv[0], VERSION, __DATE__, __TIME__);

  /* Emitters... */
  ctl->ng = (int) scan_ctl(argc, argv, "NG", -1, "0", NULL);
  if (ctl->ng < 0 || ctl->ng > NG)
    ERRMSG("Set 0 <= NG <= MAX!");
  for (int ig = 0; ig < ctl->ng; ig++)
    scan_ctl(argc, argv, "EMITTER", ig, "", ctl->emitter[ig]);

  /* Radiance channels... */
  ctl->nd = (int) scan_ctl(argc, argv, "ND", -1, "0", NULL);
  if (ctl->nd < 0 || ctl->nd > ND)
    ERRMSG("Set 0 <= ND <= MAX!");
  for (int id = 0; id < ctl->nd; id++)
    ctl->nu[id] = scan_ctl(argc, argv, "NU", id, "", NULL);

  /* Spectral windows... */
  ctl->nw = (int) scan_ctl(argc, argv, "NW", -1, "1", NULL);
  if (ctl->nw < 0 || ctl->nw > NW)
    ERRMSG("Set 0 <= NW <= MAX!");
  for (int id = 0; id < ctl->nd; id++)
    ctl->window[id] = (int) scan_ctl(argc, argv, "WINDOW", id, "0", NULL);

  /* Cloud data... */
  ctl->ncl = (int) scan_ctl(argc, argv, "NCL", -1, "0", NULL);
  if (ctl->ncl < 0 || ctl->ncl > NCL)
    ERRMSG("Set 0 <= NCL <= MAX!");
  if (ctl->ncl == 1)
    ERRMSG("Set NCL > 1!");
  for (int icl = 0; icl < ctl->ncl; icl++)
```

```
    ctl->clnu[icl] = scan_ctl(argc, argv, "CLNU", icl, "", NULL);

  /* Surface data... */
  ctl->nsf = (int) scan_ctl(argc, argv, "NSF", -1, "0", NULL);
  if (ctl->nsf < 0 || ctl->nsf > NSF)
    ERRMSG("Set 0 <= NSF <= MAX!");
  if (ctl->nsf == 1)
    ERRMSG("Set NSF > 1!");
  for (int isf = 0; isf < ctl->nsf; isf++)
    ctl->sfnu[isf] = scan_ctl(argc, argv, "SFNU", isf, "", NULL);
  ctl->sftype = (int) scan_ctl(argc, argv, "SFTYPE", -1, "2", NULL);
  if (ctl->sftype < 0 || ctl->sftype > 3)
    ERRMSG("Set 0 <= SFTYPE <= 3!");
  ctl->sfsza = scan_ctl(argc, argv, "SFSZA", -1, "-999", NULL);

  /* Emissivity look-up tables... */
  scan_ctl(argc, argv, "TBLBASE", -1, "-", ctl->tblbase);
  ctl->tblfmt = (int) scan_ctl(argc, argv, "TBLFMT", -1, "1", NULL);

  /* Hydrostatic equilibrium... */
  ctl->hydz = scan_ctl(argc, argv, "HYDZ", -1, "-999", NULL);

  /* Continua... */
  ctl->ctm_co2 = (int) scan_ctl(argc, argv, "CTM_CO2", -1, "1", NULL);
  ctl->ctm_h2o = (int) scan_ctl(argc, argv, "CTM_H2O", -1, "1", NULL);
  ctl->ctm_n2 = (int) scan_ctl(argc, argv, "CTM_N2", -1, "1", NULL);
  ctl->ctm_o2 = (int) scan_ctl(argc, argv, "CTM_O2", -1, "1", NULL);

  /* Ray-tracing... */
  ctl->refrac = (int) scan_ctl(argc, argv, "REFRAC", -1, "1", NULL);
  ctl->rayds = scan_ctl(argc, argv, "RAYDS", -1, "10", NULL);
  ctl->raydz = scan_ctl(argc, argv, "RAYDZ", -1, "0.1", NULL);

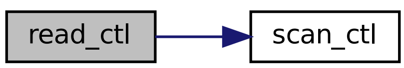
  /* Field of view... */
  scan_ctl(argc, argv, "FOV", -1, "-", ctl->fov);

  /* Retrieval interface... */
  ctl->retp_zmin = scan_ctl(argc, argv, "RETP_ZMIN", -1, "-999", NULL);
  ctl->retp_zmax = scan_ctl(argc, argv, "RETP_ZMAX", -1, "-999", NULL);
  ctl->rett_zmin = scan_ctl(argc, argv, "RETT_ZMIN", -1, "-999", NULL);
  ctl->rett_zmax = scan_ctl(argc, argv, "RETT_ZMAX", -1, "-999", NULL);
  for (int ig = 0; ig < ctl->ng; ig++) {
    ctl->retq_zmin[ig] = scan_ctl(argc, argv, "RETQ_ZMIN", ig, "-999", NULL);
    ctl->retq_zmax[ig] = scan_ctl(argc, argv, "RETQ_ZMAX", ig, "-999", NULL);
  }
  for (int iw = 0; iw < ctl->nw; iw++) {
    ctl->retk_zmin[iw] = scan_ctl(argc, argv, "RETK_ZMIN", iw, "-999", NULL);
    ctl->retk_zmax[iw] = scan_ctl(argc, argv, "RETK_ZMAX", iw, "-999", NULL);
  }
  ctl->ret_clz = (int) scan_ctl(argc, argv, "RET_CLZ", -1, "0", NULL);
  ctl->ret_cldz = (int) scan_ctl(argc, argv, "RET_CLDZ", -1, "0", NULL);
  ctl->ret_clk = (int) scan_ctl(argc, argv, "RET_CLK", -1, "0", NULL);
  ctl->ret_sfz = (int) scan_ctl(argc, argv, "RET_SFZ", -1, "0", NULL);
  ctl->ret_sfp = (int) scan_ctl(argc, argv, "RET_SFP", -1, "0", NULL);
  ctl->ret_sft = (int) scan_ctl(argc, argv, "RET_SFT", -1, "0", NULL);
  ctl->ret_sfeps = (int) scan_ctl(argc, argv, "RET_SFEPS", -1, "0", NULL);

  /* Output flags... */
  ctl->write_bbt = (int) scan_ctl(argc, argv, "WRITE_BBT", -1, "0", NULL);
  ctl->write_matrix =
    (int) scan_ctl(argc, argv, "WRITE_MATRIX", -1, "0", NULL);

  /* External forward models... */
  ctl->formod = (int) scan_ctl(argc, argv, "FORMOD", -1, "1", NULL);
  scan_ctl(argc, argv, "RFMBIN", -1, "-", ctl->rfmbin);
  scan_ctl(argc, argv, "RFMHIT", -1, "-", ctl->rfmhit);
  for (int ig = 0; ig < ctl->ng; ig++)
    scan_ctl(argc, argv, "RFMXSC", ig, "-", ctl->rfmxsc[ig]);
}
```

Here is the call graph for this function:



5.17.2.37 read_matrix()

void read_matrix (
const char * *dirname*,
const char * *filename*,
gsl_matrix * *matrix*)

Read matrix.

Definition at line 4510 of file jurassic.c.

```
                     {

  FILE *in;

  char dum[LEN], file[LEN], line[LEN];

  double value;

  int i, j;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read matrix: %s", file);

  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read data... */
  gsl_matrix_set_zero(matrix);
  while (fgets(line, LEN, in))
    if (sscanf(line, "%d %s %s %s %s %s %d %s %s %s %s %s %lg",
               &i, dum, dum, dum, dum, dum,
               &j, dum, dum, dum, dum, dum, &value) == 13)
      gsl_matrix_set(matrix, (size_t) i, (size_t) j, value);

  /* Close file... */
  fclose(in);
}
```

5.17.2.38 read_obs()

void read_obs (
const char * *dirname*,
const char * *filename*,
ctl_t * *ctl*,
obs_t * *obs*)

Read observation data.

Definition at line 4550 of file jurassic.c.

```
             {

  FILE *in;

  char file[LEN], line[LEN], *tok;

  /* Init... */
  obs->nr = 0;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read observation data: %s", file);
```

```
  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read line... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    TOK(line, tok, "%lg", obs->time[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obsz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obslon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obslat[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vpz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vplon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vplat[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tpz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tplon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tplat[obs->nr]);
    for (int id = 0; id < ctl->nd; id++)
      TOK(NULL, tok, "%lg", obs->rad[id][obs->nr]);
    for (int id = 0; id < ctl->nd; id++)
      TOK(NULL, tok, "%lg", obs->tau[id][obs->nr]);

    /* Increment counter... */
    if ((++obs->nr) > NR)
      ERRMSG("Too many rays!");
  }

  /* Close file... */
  fclose(in);

  /* Check number of points... */
  if (obs->nr < 1)
    ERRMSG("Could not read any data!");
}
```

5.17.2.39 read_obs_rfm()

```
double read_obs_rfm (
        const char * basename,
        double z,
        double * nu,
        double * f,
        int n )
```

Read observation data in RFM format.

Definition at line 4610 of file jurassic.c.

```
          {

  FILE *in;

  char filename[LEN];

  double filt, fsum = 0, nu2[NSHAPE], *nurfm, *rad, radsum = 0;

  int i, idx, ipts, npts;

  /* Allocate... */
  ALLOC(nurfm, double,
        RFMNPTS);
  ALLOC(rad, double,
        RFMNPTS);

  /* Search RFM spectrum... */
  sprintf(filename, "%s_%05d.asc", basename, (int) (z * 1000));
  if (!(in = fopen(filename, "r"))) {
    sprintf(filename, "%s_%05d.asc", basename, (int) (z * 1000) + 1);
    if (!(in = fopen(filename, "r")))
      ERRMSG("Cannot find RFM data file!");
  }
  fclose(in);

  /* Read RFM spectrum... */
  read_rfm_spec(filename, nurfm, rad, &npts);

  /* Set wavenumbers... */
  nu2[0] = nu[0];
```

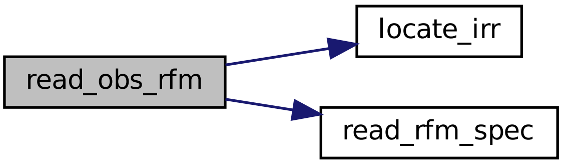
```
  nu2[n - 1] = nu[n - 1];
  for (i = 1; i < n - 1; i++)
    nu2[i] = LIN(0.0, nu2[0], n - 1.0, nu2[n - 1], i);

  /* Convolute... */
  for (ipts = 0; ipts < npts; ipts++)
    if (nurfm[ipts] >= nu2[0] && nurfm[ipts] <= nu2[n - 1]) {
      idx = locate_irr(nu2, n, nurfm[ipts]);
      filt = LIN(nu2[idx], f[idx], nu2[idx + 1], f[idx + 1], nurfm[ipts]);
      fsum += filt;
      radsum += filt * rad[ipts];
    }

  /* Free... */
  free(nurfm);
  free(rad);

  /* Return radiance... */
  return radsum / fsum;
}
```

Here is the call graph for this function:



5.17.2.40 read_rfm_spec()

```
void read_rfm_spec (
        const char * filename,
        double * nu,
        double * rad,
        int * npts )
```

Read RFM spectrum.

Definition at line 4668 of file jurassic.c.

```
                   {

  FILE *in;

  char line[RFMLINE], *tok;

  double dnu, nu0, nu1;

  int i, ipts = 0;

  /* Write info... */
  printf("Read RFM data: %s\n", filename);

  /* Open file... */
  if (!(in = fopen(filename, "r")))
    ERRMSG("Cannot open file!");

  /* Read header...... */
  for (i = 0; i < 4; i++)
    if (fgets(line, RFMLINE, in) == NULL)
      ERRMSG("Error while reading file header!");
  sscanf(line, "%d %lg %lg %lg", npts, &nu0, &dnu, &nu1);
  if (*npts > RFMNPTS)
```

```
    ERRMSG("Too many spectral grid points!");

  /* Read radiance data... */
  while (fgets(line, RFMLINE, in) && ipts < *npts - 1) {
    if ((tok = strtok(line, " \t\n")) != NULL)
      if (sscanf(tok, "%lg", &rad[ipts]) == 1)
        ipts++;
    while ((tok = strtok(NULL, " \t\n")) != NULL)
      if (sscanf(tok, "%lg", &rad[ipts]) == 1)
        ipts++;
  }
  if (ipts != *npts)
    ERRMSG("Error while reading RFM data!");

  /* Compute wavenumbers... */
  for (ipts = 0; ipts < *npts; ipts++)
    nu[ipts] = LIN(0.0, nu0, (double) (*npts - 1), nu1, (double) ipts);

  /* Close file... */
  fclose(in);
}
```

5.17.2.41 read_shape()

```
void read_shape (
    const char * filename,
    double * x,
    double * y,
    int * n )
```

Read shape function.

Definition at line 4719 of file jurassic.c.

```
                {

  FILE *in;

  char line[LEN];

  /* Write info... */
  LOG(1, "Read shape function: %s", filename);

  /* Open file... */
  if (!(in = fopen(filename, "r")))
    ERRMSG("Cannot open file!");

  /* Read data... */
  *n = 0;
  while (fgets(line, LEN, in))
    if (sscanf(line, "%lg %lg", &x[*n], &y[*n]) == 2)
      if ((++(*n)) > NSHAPE)
        ERRMSG("Too many data points!");

  /* Check number of points... */
  if (*n < 1)
    ERRMSG("Could not read any data!");

  /* Close file... */
  fclose(in);
}
```

5.17.2.42 read_tbl()

```
void read_tbl (
    ctl_t * ctl,
    tbl_t * tbl )
```

Read look-up table data.

Definition at line 4753 of file jurassic.c.

```
                        {

  FILE *in;
```

```
  char filename[2 * LEN], line[LEN];

  double eps, press, temp, u;

  /* Loop over trace gases and channels... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ig = 0; ig < ctl->ng; ig++) {

      /* Initialize... */
      tbl->np[id][ig] = -1;
      double eps_old = -999;
      double press_old = -999;
      double temp_old = -999;
      double u_old = -999;

      /* Set filename... */
      sprintf(filename, "%s_%.4f_%s.%s", ctl->tblbase,
              ctl->nu[id], ctl->emitter[ig],
              ctl->tblfmt == 1 ? "tab" : "bin");

      /* Write info... */
      LOG(1, "Read emissivity table: %s", filename);

      /* Try to open file... */
      if (!(in = fopen(filename, "r"))) {
        WARN("Missing emissivity table: %s", filename);
        continue;
      }

      /* Read ASCII tables... */
      if (ctl->tblfmt == 1) {

        /* Read data... */
        while (fgets(line, LEN, in)) {

          /* Parse line... */
          if (sscanf(line, "%lg %lg %lg %lg", &press, &temp, &u, &eps) != 4)
            continue;

          /* Check ranges... */
          if (u < 0 || u > 1e30 || eps < 0 || eps > 1)
            continue;

          /* Determine pressure index... */
          if (press != press_old) {
            press_old = press;
            if ((++tbl->np[id][ig]) >= TBLNP)
              ERRMSG("Too many pressure levels!");
            tbl->nt[id][ig][tbl->np[id][ig]] = -1;
          }

          /* Determine temperature index... */
          if (temp != temp_old) {
            temp_old = temp;
            if ((++tbl->nt[id][ig][tbl->np[id][ig]]) >= TBLNT)
              ERRMSG("Too many temperatures!");
            tbl->nu[id][ig][tbl->np[id][ig]]
              [tbl->nt[id][ig][tbl->np[id][ig]]] = -1;
          }

          /* Determine column density index... */
          if ((eps > eps_old && u > u_old) || tbl->nu[id][ig][tbl->np[id][ig]]
              [tbl->nt[id][ig][tbl->np[id][ig]]] < 0) {
            eps_old = eps;
            u_old = u;
            if ((++tbl->nu[id][ig][tbl->np[id][ig]]
                 [tbl->nt[id][ig][tbl->np[id][ig]]]) >= TBLNU) {
              tbl->nu[id][ig][tbl->np[id][ig]]
                [tbl->nt[id][ig][tbl->np[id][ig]]]--;
              continue;
            }
          }

          /* Store data... */
          tbl->p[id][ig][tbl->np[id][ig]] = press;
          tbl->t[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
            = temp;
          tbl->u[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
            [tbl->nu[id][ig][tbl->np[id][ig]]
             [tbl->nt[id][ig][tbl->np[id][ig]]]] = (float) u;
          tbl->eps[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
            [tbl->nu[id][ig][tbl->np[id][ig]]
             [tbl->nt[id][ig][tbl->np[id][ig]]]] = (float) eps;
        }

        /* Increment counters... */
```

```
          tbl->np[id][ig]++;
          for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
            tbl->nt[id][ig][ip]++;
            for (int it = 0; it < tbl->nt[id][ig][ip]; it++)
              tbl->nu[id][ig][ip][it]++;
          }
        }

        /* Read binary data... */
        else if (ctl->tblfmt == 2) {

          /* Read data... */
          FREAD(&tbl->np[id][ig], int,
                1,
                in);
          if (tbl->np[id][ig] > TBLNP)
            ERRMSG("Too many pressure levels!");
          FREAD(tbl->p[id][ig], double,
                  (size_t) tbl->np[id][ig],
                in);
          for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
            FREAD(&tbl->nt[id][ig][ip], int,
                  1,
                  in);
            if (tbl->nt[id][ig][ip] > TBLNT)
              ERRMSG("Too many temperatures!");
            FREAD(tbl->t[id][ig][ip], double,
                    (size_t) tbl->nt[id][ig][ip],
                  in);
            for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
              FREAD(&tbl->nu[id][ig][ip][it], int,
                    1,
                    in);
              if (tbl->nu[id][ig][ip][it] > TBLNU)
                ERRMSG("Too many column densities!");
              FREAD(tbl->u[id][ig][ip][it], float,
                      (size_t) tbl->nu[id][ig][ip][it],
                    in);
              FREAD(tbl->eps[id][ig][ip][it], float,
                      (size_t) tbl->nu[id][ig][ip][it],
                    in);
            }
          }
        }

        /* Error message... */
        else
          ERRMSG("Unknown look-up table format!");

        /* Close file... */
        fclose(in);
      }
}
```

5.17.2.43 refractivity()

```
double refractivity (
    double p,
    double t )
```

Compute refractivity (return value is n - 1).

Definition at line 4901 of file jurassic.c.

```
                {

  /* Refractivity of air at 4 to 15 micron... */
  return 7.753e-05 * p / t;
}
```

5.17.2.44 scan_ctl()

```
double scan_ctl (
    int argc,
    char * argv[],
    const char * varname,
```

```
int arridx,
const char * defvalue,
char * value )
```

Search control parameter file for variable entry.

Definition at line 4911 of file jurassic.c.

```
                {

  FILE *in = NULL;

  char dummy[LEN], fullname1[LEN], fullname2[LEN], line[LEN],
    rvarname[LEN], rval[LEN];

  int contain = 0;

  /* Open file... */
  if (argv[1][0] != '-')
    if (!(in = fopen(argv[1], "r")))
      ERRMSG("Cannot open file!");

  /* Set full variable name... */
  if (arridx >= 0) {
    sprintf(fullname1, "%s[%d]", varname, arridx);
    sprintf(fullname2, "%s[*]", varname);
  } else {
    sprintf(fullname1, "%s", varname);
    sprintf(fullname2, "%s", varname);
  }

  /* Read data... */
  if (in != NULL)
    while (fgets(line, LEN, in))
      if (sscanf(line, "%s %s %s", rvarname, dummy, rval) == 3)
        if (strcasecmp(rvarname, fullname1) == 0 ||
            strcasecmp(rvarname, fullname2) == 0) {
          contain = 1;
          break;
        }
  for (int i = 1; i < argc - 1; i++)
    if (strcasecmp(argv[i], fullname1) == 0 ||
        strcasecmp(argv[i], fullname2) == 0) {
      sprintf(rval, "%s", argv[i + 1]);
      contain = 1;
      break;
    }

  /* Close file... */
  if (in != NULL)
    fclose(in);

  /* Check for missing variables... */
  if (!contain) {
    if (strlen(defvalue) > 0)
      sprintf(rval, "%s", defvalue);
    else
      ERRMSG("Missing variable %s!\n", fullname1);
  }

  /* Write info... */
  LOG(1, "%s = %s", fullname1, rval);

  /* Return values... */
  if (value != NULL)
    sprintf(value, "%s", rval);
  return atof(rval);
}
```

5.17.2.45 sza()

```
double sza (
    double sec,
    double lon,
    double lat )
```

Calculate solar zenith angle.

Definition at line 4980 of file jurassic.c.

```
            {

  /* Number of days and fraction with respect to 2000-01-01T12:00Z... */
  double D = sec / 86400 - 0.5;

  /* Geocentric apparent ecliptic longitude [rad]... */
  double g = (357.529 + 0.98560028 * D) * M_PI / 180;
  double q = 280.459 + 0.98564736 * D;
  double L = (q + 1.915 * sin(g) + 0.020 * sin(2 * g)) * M_PI / 180;

  /* Mean obliquity of the ecliptic [rad]... */
  double e = (23.439 - 0.00000036 * D) * M_PI / 180;

  /* Declination [rad]... */
  double dec = asin(sin(e) * sin(L));

  /* Right ascension [rad]... */
  double ra = atan2(cos(e) * sin(L), cos(L));

  /* Greenwich Mean Sidereal Time [h]... */
  double GMST = 18.697374558 + 24.06570982441908 * D;

  /* Local Sidereal Time [h]... */
  double LST = GMST + lon / 15;

  /* Hour angle [rad]... */
  double h = LST / 12 * M_PI - ra;

  /* Convert latitude... */
  lat *= M_PI / 180;

  /* Return solar zenith angle [deg]... */
  return acos(sin(lat) * sin(dec) +
              cos(lat) * cos(dec) * cos(h)) * 180 / M_PI;
}
```

5.17.2.46 tangent_point()

```
void tangent_point (
        los_t * los,
        double * tpz,
        double * tplon,
        double * tplat )
```

Find tangent point of a given LOS.

Definition at line 5021 of file jurassic.c.

```
              {

  double dummy, v[3], v0[3], v2[3];

  /* Find minimum altitude... */
  size_t ip = gsl_stats_min_index(los->z, 1, (size_t) los->np);

  /* Nadir or zenith... */
  if (ip <= 0 || ip >= (size_t) los->np - 1) {
    *tpz = los->z[los->np - 1];
    *tplon = los->lon[los->np - 1];
    *tplat = los->lat[los->np - 1];
  }

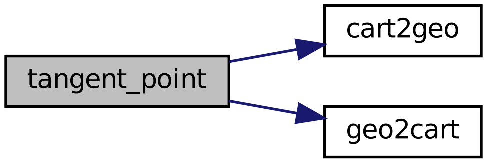
  /* Limb... */
  else {

    /* Determine interpolating polynomial y=a*x^2+b*x+c... */
    double yy0 = los->z[ip - 1];
    double yy1 = los->z[ip];
    double yy2 = los->z[ip + 1];
    double x1 = sqrt(POW2(los->ds[ip]) - POW2(yy1 - yy0));
    double x2 = x1 + sqrt(POW2(los->ds[ip + 1]) - POW2(yy2 - yy1));
    double a = 1 / (x1 - x2) * (-(yy0 - yy1) / x1 + (yy0 - yy2) / x2);
    double b = -(yy0 - yy1) / x1 - a * x1;
    double c = yy0;

    /* Get tangent point location... */
    double x = -b / (2 * a);
    *tpz = a * x * x + b * x + c;
    geo2cart(los->z[ip - 1], los->lon[ip - 1], los->lat[ip - 1], v0);
    geo2cart(los->z[ip + 1], los->lon[ip + 1], los->lat[ip + 1], v2);
```

```
    for (int i = 0; i < 3; i++)
      v[i] = LIN(0.0, v0[i], x2, v2[i], x);
    cart2geo(v, &dummy, tplon, tplat);
  }
}
```

Here is the call graph for this function:



5.17.2.47 time2jsec()

```
void time2jsec (
    int year,
    int mon,
    int day,
    int hour,
    int min,
    int sec,
    double remain,
    double * jsec )
```

Convert date to seconds.

Definition at line 5065 of file jurassic.c.

```
                  {

  struct tm t0, t1;

  t0.tm_year = 100;
  t0.tm_mon = 0;
  t0.tm_mday = 1;
  t0.tm_hour = 0;
  t0.tm_min = 0;
  t0.tm_sec = 0;

  t1.tm_year = year - 1900;
  t1.tm_mon = mon - 1;
  t1.tm_mday = day;
  t1.tm_hour = hour;
  t1.tm_min = min;
  t1.tm_sec = sec;

  *jsec = (double) timegm(&t1) - (double) timegm(&t0) + remain;
}
```

5.17.2.48 timer()

```
void timer (
    const char * name,
    const char * file,
    const char * func,
    int line,
    int mode )
```

Measure wall-clock time.

Definition at line 5096 of file jurassic.c.

```
               {

  static double w0[10];

  static int l0[10], nt;

  /* Start new timer... */
  if (mode == 1) {
    w0[nt] = omp_get_wtime();
    l0[nt] = line;
    if ((++nt) >= 10)
      ERRMSG("Too many timers!");
  }

  /* Write elapsed time... */
  else {

    /* Check timer index... */
    if (nt - 1 < 0)
      ERRMSG("Coding error!");

    /* Write elapsed time... */
    LOG(1, "Timer '%s' (%s, %s, l%d-%d): %.3f sec",
        name, file, func, l0[nt - 1], line, omp_get_wtime() - w0[nt - 1]);
  }

  /* Stop timer... */
  if (mode == 3)
    nt--;
}
```

5.17.2.49 write_atm()

```
void write_atm (
    const char * dirname,
    const char * filename,
    ctl_t * ctl,
    atm_t * atm )
```

Write atmospheric data.

Definition at line 5134 of file jurassic.c.

```
                  {

  FILE *out;

  char file[LEN];

  int n = 6;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write atmospheric data: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
```

```
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = altitude [km]\n"
          "# $3 = longitude [deg]\n"
          "# $4 = latitude [deg]\n"
          "# $5 = pressure [hPa]\n" "# $6 = temperature [K]\n");
  for (int ig = 0; ig < ctl->ng; ig++)
    fprintf(out, "# $%d = %s volume mixing ratio [ppv]\n",
            ++n, ctl->emitter[ig]);
  for (int iw = 0; iw < ctl->nw; iw++)
    fprintf(out, "# $%d = extinction (window %d) [1/km]\n", ++n, iw);
  if (ctl->ncl > 0) {
    fprintf(out, "# $%d = cloud layer height [km]\n", ++n);
    fprintf(out, "# $%d = cloud layer depth [km]\n", ++n);
    for (int icl = 0; icl < ctl->ncl; icl++)
      fprintf(out, "# $%d = cloud layer extinction (%.4f cm^-1) [1/km]\n",
              ++n, ctl->clnu[icl]);
  }
  if (ctl->nsf > 0) {
    fprintf(out, "# $%d = surface layer height [km]\n", ++n);
    fprintf(out, "# $%d = surface layer pressure [hPa]\n", ++n);
    fprintf(out, "# $%d = surface layer temperature [K]\n", ++n);
    for (int isf = 0; isf < ctl->nsf; isf++)
      fprintf(out, "# $%d = surface layer emissivity (%.4f cm^-1)\n",
              ++n, ctl->sfnu[isf]);
  }

  /* Write data... */
  for (int ip = 0; ip < atm->np; ip++) {
    if (ip == 0 || atm->time[ip] != atm->time[ip - 1])
      fprintf(out, "\n");
    fprintf(out, "%.2f %g %g %g %g %g", atm->time[ip], atm->z[ip],
            atm->lon[ip], atm->lat[ip], atm->p[ip], atm->t[ip]);
    for (int ig = 0; ig < ctl->ng; ig++)
      fprintf(out, " %g", atm->q[ig][ip]);
    for (int iw = 0; iw < ctl->nw; iw++)
      fprintf(out, " %g", atm->k[iw][ip]);
    if (ctl->ncl > 0) {
      fprintf(out, " %g %g", atm->clz, atm->cldz);
      for (int icl = 0; icl < ctl->ncl; icl++)
        fprintf(out, " %g", atm->clk[icl]);
    }
    if (ctl->nsf > 0) {
      fprintf(out, " %g %g %g", atm->sfz, atm->sfp, atm->sft);
      for (int isf = 0; isf < ctl->nsf; isf++)
        fprintf(out, " %g", atm->sfeps[isf]);
    }
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);
}
```

5.17.2.50 write_atm_rfm()

```
void write_atm_rfm (
    const char * filename,
    ctl_t * ctl,
    atm_t * atm )
```

Write atmospheric data in RFM format.

Definition at line 5216 of file jurassic.c.

```
                    {

  FILE *out;

  int ig, ip;

  /* Write info... */
  printf("Write RFM data: %s\n", filename);

  /* Create file... */
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create file!");

  /* Write data... */
  fprintf(out, "%d\n", atm->np);
  fprintf(out, "*HGT [km]\n");
  for (ip = 0; ip < atm->np; ip++)
```

```
05236     fprintf(out, "%g\n", atm->z[ip]);
05237   fprintf(out, "*PRE [mb]\n");
05238   for (ip = 0; ip < atm->np; ip++)
05239     fprintf(out, "%g\n", atm->p[ip]);
05240   fprintf(out, "*TEM [K]\n");
05241   for (ip = 0; ip < atm->np; ip++)
05242     fprintf(out, "%g\n", atm->t[ip]);
05243   for (ig = 0; ig < ctl->ng; ig++) {
05244     fprintf(out, "*%s [ppmv]\n", ctl->emitter[ig]);
05245     for (ip = 0; ip < atm->np; ip++)
05246       fprintf(out, "%g\n", atm->q[ig][ip] * 1e6);
05247   }
05248   fprintf(out, "*END\n");
05249
05250   /* Close file... */
05251   fclose(out);
05252 }
```

5.17.2.51 write_matrix()

```
void write_matrix (
    const char * dirname,
    const char * filename,
    ctl_t * ctl,
    gsl_matrix * matrix,
    atm_t * atm,
    obs_t * obs,
    const char * rowspace,
    const char * colspace,
    const char * sort )
```

Write matrix.

Definition at line 5256 of file jurassic.c.

```
05265                     {
05266
05267   FILE *out;
05268
05269   char file[LEN], quantity[LEN];
05270
05271   int *cida, *ciqa, *cipa, *cira, *rida, *riqa, *ripa, *rira;
05272
05273   size_t i, j, nc, nr;
05274
05275   /* Check output flag... */
05276   if (!ctl->write_matrix)
05277     return;
05278
05279   /* Allocate... */
05280   ALLOC(cida, int,
05281         M);
05282   ALLOC(ciqa, int,
05283         N);
05284   ALLOC(cipa, int,
05285         N);
05286   ALLOC(cira, int,
05287         M);
05288   ALLOC(rida, int,
05289         M);
05290   ALLOC(riqa, int,
05291         N);
05292   ALLOC(ripa, int,
05293         N);
05294   ALLOC(rira, int,
05295         M);
05296
05297   /* Set filename... */
05298   if (dirname != NULL)
05299     sprintf(file, "%s/%s", dirname, filename);
05300   else
05301     sprintf(file, "%s", filename);
05302
05303   /* Write info... */
05304   LOG(1, "Write matrix: %s", file);
05305
05306   /* Create file... */
05307   if (!(out = fopen(file, "w")))
```

```
    ERRMSG("Cannot create file!");

  /* Write header (row space)... */
  if (rowspace[0] == 'y') {

    fprintf(out,
            "# $1 = Row: index (measurement space)\n"
            "# $2 = Row: channel wavenumber [cm^-1]\n"
            "# $3 = Row: time (seconds since 2000-01-01T00:00Z)\n"
            "# $4 = Row: view point altitude [km]\n"
            "# $5 = Row: view point longitude [deg]\n"
            "# $6 = Row: view point latitude [deg]\n");

    /* Get number of rows... */
    nr = obs2y(ctl, obs, NULL, rida, rira);

  } else {

    fprintf(out,
            "# $1 = Row: index (state space)\n"
            "# $2 = Row: name of quantity\n"
            "# $3 = Row: time (seconds since 2000-01-01T00:00Z)\n"
            "# $4 = Row: altitude [km]\n"
            "# $5 = Row: longitude [deg]\n" "# $6 = Row: latitude [deg]\n");

    /* Get number of rows... */
    nr = atm2x(ctl, atm, NULL, riqa, ripa);
  }

  /* Write header (column space)... */
  if (colspace[0] == 'y') {

    fprintf(out,
            "# $7 = Col: index (measurement space)\n"
            "# $8 = Col: channel wavenumber [cm^-1]\n"
            "# $9 = Col: time (seconds since 2000-01-01T00:00Z)\n"
            "# $10 = Col: view point altitude [km]\n"
            "# $11 = Col: view point longitude [deg]\n"
            "# $12 = Col: view point latitude [deg]\n");

    /* Get number of columns... */
    nc = obs2y(ctl, obs, NULL, cida, cira);

  } else {

    fprintf(out,
            "# $7 = Col: index (state space)\n"
            "# $8 = Col: name of quantity\n"
            "# $9 = Col: time (seconds since 2000-01-01T00:00Z)\n"
            "# $10 = Col: altitude [km]\n"
            "# $11 = Col: longitude [deg]\n" "# $12 = Col: latitude [deg]\n");

    /* Get number of columns... */
    nc = atm2x(ctl, atm, NULL, ciqa, cipa);
  }

  /* Write header entry... */
  fprintf(out, "# $13 = Matrix element\n\n");

  /* Write matrix data... */
  i = j = 0;
  while (i < nr && j < nc) {

    /* Write info about the row... */
    if (rowspace[0] == 'y')
      fprintf(out, "%d %.4f %.2f %g %g %g",
              (int) i, ctl->nu[rida[i]],
              obs->time[rira[i]], obs->vpz[rira[i]],
              obs->vplon[rira[i]], obs->vplat[rira[i]]);
    else {
      idx2name(ctl, riqa[i], quantity);
      fprintf(out, "%d %s %.2f %g %g %g", (int) i, quantity,
              atm->time[ripa[i]], atm->z[ripa[i]],
              atm->lon[ripa[i]], atm->lat[ripa[i]]);
    }

    /* Write info about the column... */
    if (colspace[0] == 'y')
      fprintf(out, " %d %.4f %.2f %g %g %g",
              (int) j, ctl->nu[cida[j]],
              obs->time[cira[j]], obs->vpz[cira[j]],
              obs->vplon[cira[j]], obs->vplat[cira[j]]);
    else {
      idx2name(ctl, ciqa[j], quantity);
      fprintf(out, " %d %s %.2f %g %g %g", (int) j, quantity,
              atm->time[cipa[j]], atm->z[cipa[j]],
              atm->lon[cipa[j]], atm->lat[cipa[j]]);
```

```
    }

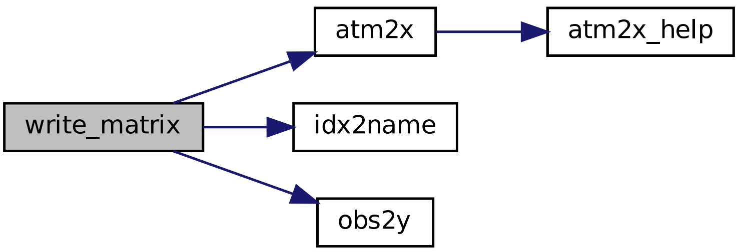
    /* Write matrix entry... */
    fprintf(out, " %g\n", gsl_matrix_get(matrix, i, j));

    /* Set matrix indices... */
    if (sort[0] == 'r') {
      j++;
      if (j >= nc) {
        j = 0;
        i++;
        fprintf(out, "\n");
      }
    } else {
      i++;
      if (i >= nr) {
        i = 0;
        j++;
        fprintf(out, "\n");
      }
    }
  }

  /* Close file... */
  fclose(out);

  /* Free... */
  free(cida);
  free(ciqa);
  free(cipa);
  free(cira);
  free(rida);
  free(riqa);
  free(ripa);
  free(rira);
}
```

Here is the call graph for this function:



5.17.2.52 write_obs()

```
void write_obs (
    const char * dirname,
    const char * filename,
    ctl_t * ctl,
    obs_t * obs )
```

Write observation data.

Definition at line 5434 of file jurassic.c.

```
               {

  FILE *out;
```

```
  char file[LEN];

  int n = 10;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write observation data: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n");
  for (int id = 0; id < ctl->nd; id++)
    fprintf(out, "# $%d = radiance (%.4f cm^-1) [W/(m^2 sr cm^-1)]\n",
            ++n, ctl->nu[id]);
  for (int id = 0; id < ctl->nd; id++)
    fprintf(out, "# $%d = transmittance (%.4f cm^-1) [-]\n", ++n,
            ctl->nu[id]);

  /* Write data... */
  for (int ir = 0; ir < obs->nr; ir++) {
    if (ir == 0 || obs->time[ir] != obs->time[ir - 1])
      fprintf(out, "\n");
    fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g", obs->time[ir],
            obs->obsz[ir], obs->obslon[ir], obs->obslat[ir],
            obs->vpz[ir], obs->vplon[ir], obs->vplat[ir],
            obs->tpz[ir], obs->tplon[ir], obs->tplat[ir]);
    for (int id = 0; id < ctl->nd; id++)
      fprintf(out, " %g", obs->rad[id][ir]);
    for (int id = 0; id < ctl->nd; id++)
      fprintf(out, " %g", obs->tau[id][ir]);
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);
}
```

5.17.2.53 write_shape()

```
void write_shape (
    const char * filename,
    double * x,
    double * y,
    int n )
```

Write shape function.

Definition at line 5499 of file jurassic.c.

```
        {

  FILE *out;

  /* Write info... */
  LOG(1, "Write shape function: %s", filename);

  /* Create file... */
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
```

```
  fprintf(out,
          "# $1 = shape function x-value [-]\n"
          "# $2 = shape function y-value [-]\n\n");

  /* Write data... */
  for (int i = 0; i < n; i++)
    fprintf(out, "%.10g %.10g\n", x[i], y[i]);

  /* Close file... */
  fclose(out);
}
```

5.17.2.54 write_tbl() void write_tbl (ctl_t * ctl, tbl_t * tbl)

Write look-up table data.

Definition at line 5529 of file jurassic.c.

```
                    {

  FILE *out;

  char filename[2 * LEN];

  /* Loop over emitters and detectors... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int id = 0; id < ctl->nd; id++) {

      /* Set filename... */
      sprintf(filename, "%s_%.4f_%s.%s", ctl->tblbase,
              ctl->nu[id], ctl->emitter[ig],
              ctl->tblfmt == 1 ? "tab" : "bin");

      /* Write info... */
      LOG(1, "Write emissivity table: %s", filename);

      /* Create file... */
      if (!(out = fopen(filename, "w")))
        ERRMSG("Cannot create file!");

      /* Write ASCII data... */
      if (ctl->tblfmt == 1) {

        /* Write header... */
        fprintf(out,
                "# $1 = pressure [hPa]\n"
                "# $2 = temperature [K]\n"
                "# $3 = column density [molecules/cm^2]\n"
                "# $4 = emissivity [-]\n");

        /* Save table file... */
        for (int ip = 0; ip < tbl->np[id][ig]; ip++)
          for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
            fprintf(out, "\n");
            for (int iu = 0; iu < tbl->nu[id][ig][ip][it]; iu++)
              fprintf(out, "%g %g %e %e\n",
                      tbl->p[id][ig][ip], tbl->t[id][ig][ip][it],
                      tbl->u[id][ig][ip][it][iu],
                      tbl->eps[id][ig][ip][it][iu]);
          }
      }

      /* Write binary data... */
      else if (ctl->tblfmt == 2) {
        FWRITE(&tbl->np[id][ig], int,
               1,
               out);
        FWRITE(tbl->p[id][ig], double,
                 (size_t) tbl->np[id][ig],
               out);
        for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
          FWRITE(&tbl->nt[id][ig][ip], int,
                 1,
                 out);
          FWRITE(tbl->t[id][ig][ip], double,
                   (size_t) tbl->nt[id][ig][ip],
                 out);
```

```
          for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
            FWRITE(&tbl->nu[id][ig][ip][it], int,
                   1,
                   out);
            FWRITE(tbl->u[id][ig][ip][it], float,
                     (size_t) tbl->nu[id][ig][ip][it],
                   out);
            FWRITE(tbl->eps[id][ig][ip][it], float,
                     (size_t) tbl->nu[id][ig][ip][it],
                   out);
          }
        }
      }

      /* Error message... */
      else
        ERRMSG("Unknown look-up table format!");

      /* Close file... */
      fclose(out);
    }
}
```

5.17.2.55 x2atm()

```
void x2atm (
    ctl_t * ctl,
    gsl_vector * x,
    atm_t * atm )
```

Decompose parameter vector or state vector.

Definition at line 5615 of file jurassic.c.

```
                     {

  size_t n = 0;

  /* Get pressure... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->retp_zmin && atm->z[ip] <= ctl->retp_zmax)
      x2atm_help(&atm->p[ip], x, &n);

  /* Get temperature... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->rett_zmin && atm->z[ip] <= ctl->rett_zmax)
      x2atm_help(&atm->t[ip], x, &n);

  /* Get volume mixing ratio... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retq_zmin[ig]
          && atm->z[ip] <= ctl->retq_zmax[ig])
        x2atm_help(&atm->q[ig][ip], x, &n);

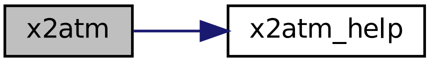
  /* Get extinction... */
  for (int iw = 0; iw < ctl->nw; iw++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retk_zmin[iw]
          && atm->z[ip] <= ctl->retk_zmax[iw])
        x2atm_help(&atm->k[iw][ip], x, &n);

  /* Get cloud data... */
  if (ctl->ret_clz)
    x2atm_help(&atm->clz, x, &n);
  if (ctl->ret_cldz)
    x2atm_help(&atm->cldz, x, &n);
  if (ctl->ret_clk)
    for (int icl = 0; icl < ctl->ncl; icl++)
      x2atm_help(&atm->clk[icl], x, &n);

  /* Get surface data... */
  if (ctl->ret_sfz)
    x2atm_help(&atm->sfz, x, &n);
  if (ctl->ret_sfp)
    x2atm_help(&atm->sfp, x, &n);
  if (ctl->ret_sft)
    x2atm_help(&atm->sft, x, &n);
  if (ctl->ret_sfeps)
    for (int isf = 0; isf < ctl->nsf; isf++)
      x2atm_help(&atm->sfeps[isf], x, &n);
```

```
}
```

Here is the call graph for this function:



5.17.2.56 x2atm_help()

```
void x2atm_help (
    double * value,
    gsl_vector * x,
    size_t * n )
```

Get element from state vector.

Definition at line 5669 of file jurassic.c.

```
                 {

  /* Get state vector element... */
  *value = gsl_vector_get(x, *n);
  (*n)++;
}
```

5.17.2.57 y2obs()

```
void y2obs (
    ctl_t * ctl,
    gsl_vector * y,
    obs_t * obs )
```

Decompose measurement vector.

Definition at line 5681 of file jurassic.c.

```
                  {

  size_t m = 0;

  /* Decompose measurement vector... */
  for (int ir = 0; ir < obs->nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      if (gsl_finite(obs->rad[id][ir])) {
        obs->rad[id][ir] = gsl_vector_get(y, m);
        m++;
      }
}
```

5.18 jurassic.c

```
/*
  This file is part of JURASSIC.

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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

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  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

/*****************************************************************************/

size_t atm2x(
  ctl_t * ctl,
  atm_t * atm,
  gsl_vector * x,
  int *iqa,
  int *ipa) {

  size_t n = 0;

  /* Add pressure... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->retp_zmin && atm->z[ip] <= ctl->retp_zmax)
      atm2x_help(atm->p[ip], IDXP, ip, x, iqa, ipa, &n);

  /* Add temperature... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->rett_zmin && atm->z[ip] <= ctl->rett_zmax)
      atm2x_help(atm->t[ip], IDXT, ip, x, iqa, ipa, &n);

  /* Add volume mixing ratios... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retq_zmin[ig]
          && atm->z[ip] <= ctl->retq_zmax[ig])
        atm2x_help(atm->q[ig][ip], IDXQ(ig), ip, x, iqa, ipa, &n);

  /* Add extinction... */
  for (int iw = 0; iw < ctl->nw; iw++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retk_zmin[iw]
          && atm->z[ip] <= ctl->retk_zmax[iw])
        atm2x_help(atm->k[iw][ip], IDXK(iw), ip, x, iqa, ipa, &n);

  /* Add cloud parameters... */
  if (ctl->ret_clz)
    atm2x_help(atm->clz, IDXCLZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_cldz)
    atm2x_help(atm->cldz, IDXCLDZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_clk)
    for (int icl = 0; icl < ctl->ncl; icl++)
      atm2x_help(atm->clk[icl], IDXCLK(icl), 0, x, iqa, ipa, &n);

  /* Add surface parameters... */
  if (ctl->ret_sfz)
    atm2x_help(atm->sfz, IDXSFZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_sfp)
    atm2x_help(atm->sfp, IDXSFP, 0, x, iqa, ipa, &n);
  if (ctl->ret_sft)
    atm2x_help(atm->sft, IDXSFT, 0, x, iqa, ipa, &n);
  if (ctl->ret_sfeps)
    for (int isf = 0; isf < ctl->nsf; isf++)
      atm2x_help(atm->sfeps[isf], IDXSFEPS(isf), 0, x, iqa, ipa, &n);

  return n;
}

/*****************************************************************************/

void atm2x_help(
  double value,
  int value_iqa,
  int value_ip,
```

```
  gsl_vector * x,
  int *iqa,
  int *ipa,
  size_t *n) {

  /* Add element to state vector... */
  if (x != NULL)
    gsl_vector_set(x, *n, value);
  if (iqa != NULL)
    iqa[*n] = value_iqa;
  if (ipa != NULL)
    ipa[*n] = value_ip;
  (*n)++;
}


/*****************************************************************************/

double brightness(
  double rad,
  double nu) {

  return C2 * nu / gsl_log1p(C1 * POW3(nu) / rad);
}


/*****************************************************************************/

void cart2geo(
  double *x,
  double *z,
  double *lon,
  double *lat) {

  double radius = NORM(x);

  *lat = asin(x[2] / radius) * 180 / M_PI;
  *lon = atan2(x[1], x[0]) * 180 / M_PI;
  *z = radius - RE;
}

/*****************************************************************************/

void climatology(
  ctl_t * ctl,
  atm_t * atm) {

  static double z[121] = {
    0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,
    20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37,
    38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55,
    56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73,
    74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91,
    92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107,
    108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120
  };

  static double pre[121] = {
    1017, 901.083, 796.45, 702.227, 617.614, 541.644, 473.437, 412.288,
    357.603, 308.96, 265.994, 228.348, 195.619, 167.351, 143.039, 122.198,
    104.369, 89.141, 76.1528, 65.0804, 55.641, 47.591, 40.7233, 34.8637,
    29.8633, 25.5956, 21.9534, 18.8445, 16.1909, 13.9258, 11.9913,
    10.34, 8.92988, 7.72454, 6.6924, 5.80701, 5.04654, 4.39238, 3.82902,
    3.34337, 2.92413, 2.56128, 2.2464, 1.97258, 1.73384, 1.52519, 1.34242,
    1.18197, 1.04086, 0.916546, 0.806832, 0.709875, 0.624101, 0.548176,
    0.480974, 0.421507, 0.368904, 0.322408, 0.281386, 0.245249, 0.213465,
    0.185549, 0.161072, 0.139644, 0.120913, 0.104568, 0.0903249, 0.0779269,
    0.0671493, 0.0577962, 0.0496902, 0.0426736, 0.0366093, 0.0313743,
    0.0268598, 0.0229699, 0.0196206, 0.0167399, 0.0142646, 0.0121397,
    0.0103181, 0.00875775, 0.00742226, 0.00628076, 0.00530519, 0.00447183,
    0.00376124, 0.00315632, 0.00264248, 0.00220738, 0.00184003, 0.00153095,
    0.00127204, 0.00105608, 0.000876652, 0.00072798, 0.00060492,
    0.000503201, 0.000419226, 0.000349896, 0.000292659, 0.000245421,
    0.000206394, 0.000174125, 0.000147441, 0.000125333, 0.000106985,
    9.173e-05, 7.90172e-05, 6.84172e-05, 5.95574e-05, 5.21183e-05,
    4.58348e-05, 4.05127e-05, 3.59987e-05, 3.21583e-05, 2.88718e-05,
    2.60322e-05, 2.35687e-05, 2.14263e-05, 1.95489e-05
  };

  static double tem[121] = {
    285.14, 279.34, 273.91, 268.3, 263.24, 256.55, 250.2, 242.82, 236.17,
    229.87, 225.04, 221.19, 218.85, 217.19, 216.2, 215.68, 215.42, 215.55,
    215.92, 216.4, 216.93, 217.45, 218, 218.68, 219.39, 220.25, 221.3,
    222.41, 223.88, 225.42, 227.2, 229.52, 231.89, 234.51, 236.85, 239.42,
    241.94, 244.57, 247.36, 250.32, 253.34, 255.82, 258.27, 260.39,
    262.03, 263.45, 264.2, 264.78, 264.67, 264.38, 263.24, 262.03, 260.02,
    258.09, 255.63, 253.28, 250.43, 247.81, 245.26, 242.77, 240.38,
```

```
  237.94, 235.79, 233.53, 231.5, 229.53, 227.6, 225.62, 223.77, 222.06,
  220.33, 218.69, 217.18, 215.64, 214.13, 212.52, 210.86, 209.25,
  207.49, 205.81, 204.11, 202.22, 200.32, 198.39, 195.92, 193.46,
  190.94, 188.31, 185.82, 183.57, 181.43, 179.74, 178.64, 178.1, 178.25,
  178.7, 179.41, 180.67, 182.31, 184.18, 186.6, 189.53, 192.66, 196.54,
  201.13, 205.93, 211.73, 217.86, 225, 233.53, 242.57, 252.14, 261.48,
  272.97, 285.26, 299.12, 312.2, 324.17, 338.34, 352.56, 365.28
};

static double c2h2[121] = {
  1.352e-09, 2.83e-10, 1.269e-10, 6.926e-11, 4.346e-11, 2.909e-11,
  2.014e-11, 1.363e-11, 8.71e-12, 5.237e-12, 2.718e-12, 1.375e-12,
  5.786e-13, 2.16e-13, 7.317e-14, 2.551e-14, 1.055e-14, 4.758e-15,
  2.056e-15, 7.703e-16, 2.82e-16, 1.035e-16, 4.382e-17, 1.946e-17,
  9.638e-18, 5.2e-18, 2.811e-18, 1.494e-18, 7.925e-19, 4.213e-19,
  1.998e-19, 8.78e-20, 3.877e-20, 1.728e-20, 7.743e-21, 3.536e-21,
  1.623e-21, 7.508e-22, 3.508e-22, 1.65e-22, 7.837e-23, 3.733e-23,
  1.808e-23, 8.77e-24, 4.285e-24, 2.095e-24, 1.032e-24, 5.082e-25,
  2.506e-25, 1.236e-25, 6.088e-26, 2.996e-26, 1.465e-26, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
};

static double c2h6[121] = {
  2.667e-09, 2.02e-09, 1.658e-09, 1.404e-09, 1.234e-09, 1.109e-09,
  1.012e-09, 9.262e-10, 8.472e-10, 7.71e-10, 6.932e-10, 6.216e-10,
  5.503e-10, 4.87e-10, 4.342e-10, 3.861e-10, 3.347e-10, 2.772e-10,
  2.209e-10, 1.672e-10, 1.197e-10, 8.536e-11, 5.783e-11, 3.846e-11,
  2.495e-11, 1.592e-11, 1.017e-11, 6.327e-12, 3.895e-12, 2.403e-12,
  1.416e-12, 8.101e-13, 4.649e-13, 2.686e-13, 1.557e-13, 9.14e-14,
  5.386e-14, 3.19e-14, 1.903e-14, 1.14e-14, 6.875e-15, 4.154e-15,
  2.538e-15, 1.553e-15, 9.548e-16, 5.872e-16, 3.63e-16, 2.244e-16,
  1.388e-16, 8.587e-17, 5.308e-17, 3.279e-17, 2.017e-17, 1.238e-17,
  7.542e-18, 4.585e-18, 2.776e-18, 1.671e-18, 9.985e-19, 5.937e-19,
  3.518e-19, 2.07e-19, 1.215e-19, 7.06e-20, 4.097e-20, 2.37e-20,
  1.363e-20, 7.802e-21, 4.441e-21, 2.523e-21, 1.424e-21, 8.015e-22,
  4.497e-22, 2.505e-22, 1.391e-22, 7.691e-23, 4.238e-23, 2.331e-23,
  1.274e-23, 6.929e-24, 3.752e-24, 2.02e-24, 1.083e-24, 5.774e-25,
  3.041e-25, 1.593e-25, 8.308e-26, 4.299e-26, 2.195e-26, 1.112e-26,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0
};

static double ccl4[121] = {
  1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10,
  1.075e-10, 1.075e-10, 1.075e-10, 1.06e-10, 1.024e-10, 9.69e-11,
  8.93e-11, 8.078e-11, 7.213e-11, 6.307e-11, 5.383e-11, 4.49e-11,
  3.609e-11, 2.705e-11, 1.935e-11, 1.385e-11, 8.35e-12, 5.485e-12,
  3.853e-12, 2.22e-12, 5.875e-13, 3.445e-13, 1.015e-13, 6.075e-14,
  4.383e-14, 2.692e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
  1e-14, 1e-14, 1e-14
};

static double ch4[121] = {
  1.864e-06, 1.835e-06, 1.819e-06, 1.805e-06, 1.796e-06, 1.788e-06,
  1.782e-06, 1.776e-06, 1.769e-06, 1.761e-06, 1.749e-06, 1.734e-06,
  1.716e-06, 1.692e-06, 1.654e-06, 1.61e-06, 1.567e-06, 1.502e-06,
  1.433e-06, 1.371e-06, 1.323e-06, 1.277e-06, 1.232e-06, 1.188e-06,
  1.147e-06, 1.108e-06, 1.07e-06, 1.027e-06, 9.854e-07, 9.416e-07,
  8.933e-07, 8.478e-07, 7.988e-07, 7.515e-07, 7.07e-07, 6.64e-07,
  6.239e-07, 5.864e-07, 5.512e-07, 5.184e-07, 4.87e-07, 4.571e-07,
  4.296e-07, 4.04e-07, 3.802e-07, 3.578e-07, 3.383e-07, 3.203e-07,
  3.032e-07, 2.889e-07, 2.76e-07, 2.635e-07, 2.519e-07, 2.409e-07,
  2.302e-07, 2.219e-07, 2.144e-07, 2.071e-07, 1.999e-07, 1.93e-07,
  1.862e-07, 1.795e-07, 1.731e-07, 1.668e-07, 1.607e-07, 1.548e-07,
  1.49e-07, 1.434e-07, 1.38e-07, 1.328e-07, 1.277e-07, 1.227e-07,
  1.18e-07, 1.134e-07, 1.089e-07, 1.046e-07, 1.004e-07, 9.635e-08,
  9.245e-08, 8.867e-08, 8.502e-08, 8.15e-08, 7.809e-08, 7.48e-08,
  7.159e-08, 6.849e-08, 6.55e-08, 6.262e-08, 5.98e-08, 5.708e-08,
  5.448e-08, 5.194e-08, 4.951e-08, 4.72e-08, 4.5e-08, 4.291e-08,
  4.093e-08, 3.905e-08, 3.729e-08, 3.563e-08, 3.408e-08, 3.265e-08,
  3.128e-08, 2.996e-08, 2.87e-08, 2.76e-08, 2.657e-08, 2.558e-08,
  2.467e-08, 2.385e-08, 2.307e-08, 2.234e-08, 2.168e-08, 2.108e-08,
  2.05e-08, 1.998e-08, 1.947e-08, 1.902e-08, 1.86e-08, 1.819e-08,
  1.782e-08
};

static double clo[121] = {
```

```
  7.419e-15, 1.061e-14, 1.518e-14, 2.195e-14, 3.175e-14, 4.666e-14,
  6.872e-14, 1.03e-13, 1.553e-13, 2.375e-13, 3.664e-13, 5.684e-13,
  8.915e-13, 1.402e-12, 2.269e-12, 4.125e-12, 7.501e-12, 1.257e-11,
  2.048e-11, 3.338e-11, 5.44e-11, 8.846e-11, 1.008e-10, 1.082e-10,
  1.157e-10, 1.232e-10, 1.312e-10, 1.539e-10, 1.822e-10, 2.118e-10,
  2.387e-10, 2.687e-10, 2.875e-10, 3.031e-10, 3.23e-10, 3.648e-10,
  4.117e-10, 4.477e-10, 4.633e-10, 4.794e-10, 4.95e-10, 5.104e-10,
  5.259e-10, 5.062e-10, 4.742e-10, 4.443e-10, 4.051e-10, 3.659e-10,
  3.305e-10, 2.911e-10, 2.54e-10, 2.215e-10, 1.927e-10, 1.675e-10,
  1.452e-10, 1.259e-10, 1.09e-10, 9.416e-11, 8.119e-11, 6.991e-11,
  6.015e-11, 5.163e-11, 4.43e-11, 3.789e-11, 3.24e-11, 2.769e-11,
  2.361e-11, 2.011e-11, 1.71e-11, 1.453e-11, 1.233e-11, 1.045e-11,
  8.851e-12, 7.48e-12, 6.316e-12, 5.326e-12, 4.487e-12, 3.778e-12,
  3.176e-12, 2.665e-12, 2.234e-12, 1.87e-12, 1.563e-12, 1.304e-12,
  1.085e-12, 9.007e-13, 7.468e-13, 6.179e-13, 5.092e-13, 4.188e-13,
  3.442e-13, 2.816e-13, 2.304e-13, 1.885e-13, 1.542e-13, 1.263e-13,
  1.035e-13, 8.5e-14, 7.004e-14, 5.783e-14, 4.795e-14, 4.007e-14,
  3.345e-14, 2.792e-14, 2.33e-14, 1.978e-14, 1.686e-14, 1.438e-14,
  1.234e-14, 1.07e-14, 9.312e-15, 8.131e-15, 7.164e-15, 6.367e-15,
  5.67e-15, 5.088e-15, 4.565e-15, 4.138e-15, 3.769e-15, 3.432e-15,
  3.148e-15
};

static double clono2[121] = {
  1.011e-13, 1.515e-13, 2.272e-13, 3.446e-13, 5.231e-13, 8.085e-13,
  1.253e-12, 1.979e-12, 3.149e-12, 5.092e-12, 8.312e-12, 1.366e-11,
  2.272e-11, 3.791e-11, 6.209e-11, 9.101e-11, 1.334e-10, 1.951e-10,
  2.853e-10, 3.94e-10, 4.771e-10, 5.771e-10, 6.675e-10, 7.665e-10,
  8.504e-10, 8.924e-10, 9.363e-10, 8.923e-10, 8.411e-10, 7.646e-10,
  6.525e-10, 5.576e-10, 4.398e-10, 3.403e-10, 2.612e-10, 1.915e-10,
  1.407e-10, 1.028e-10, 7.455e-11, 5.42e-11, 3.708e-11, 2.438e-11,
  1.618e-11, 1.075e-11, 7.17e-12, 4.784e-12, 3.205e-12, 2.147e-12,
  1.44e-12, 9.654e-13, 6.469e-13, 4.332e-13, 2.891e-13, 1.926e-13,
  1.274e-13, 8.422e-14, 5.547e-14, 3.636e-14, 2.368e-14, 1.536e-14,
  9.937e-15, 6.39e-15, 4.101e-15, 2.61e-15, 1.659e-15, 1.052e-15,
  6.638e-16, 4.172e-16, 2.61e-16, 1.63e-16, 1.013e-16, 6.275e-17,
  3.879e-17, 2.383e-17, 1.461e-17, 8.918e-18, 5.43e-18, 3.301e-18,
  1.997e-18, 1.203e-18, 7.216e-19, 4.311e-19, 2.564e-19, 1.519e-19,
  8.911e-20, 5.203e-20, 3.026e-20, 1.748e-20, 9.99e-21, 5.673e-21,
  3.215e-21, 1.799e-21, 1.006e-21, 5.628e-22, 3.146e-22, 1.766e-22,
  9.94e-23, 5.614e-23, 3.206e-23, 1.841e-23, 1.071e-23, 6.366e-24,
  3.776e-24, 2.238e-24, 1.326e-24, 8.253e-25, 5.201e-25, 3.279e-25,
  2.108e-25, 1.395e-25, 9.326e-26, 6.299e-26, 4.365e-26, 3.104e-26,
  2.219e-26, 1.621e-26, 1.185e-26, 8.92e-27, 6.804e-27, 5.191e-27,
  4.041e-27
};

static double co[121] = {
  1.907e-07, 1.553e-07, 1.362e-07, 1.216e-07, 1.114e-07, 1.036e-07,
  9.737e-08, 9.152e-08, 8.559e-08, 7.966e-08, 7.277e-08, 6.615e-08,
  5.884e-08, 5.22e-08, 4.699e-08, 4.284e-08, 3.776e-08, 3.274e-08,
  2.845e-08, 2.479e-08, 2.246e-08, 2.054e-08, 1.991e-08, 1.951e-08,
  1.94e-08, 2.009e-08, 2.1e-08, 2.201e-08, 2.322e-08, 2.45e-08,
  2.602e-08, 2.73e-08, 2.867e-08, 2.998e-08, 3.135e-08, 3.255e-08,
  3.352e-08, 3.426e-08, 3.484e-08, 3.53e-08, 3.593e-08, 3.671e-08,
  3.759e-08, 3.945e-08, 4.192e-08, 4.49e-08, 5.03e-08, 5.703e-08,
  6.538e-08, 7.878e-08, 9.644e-08, 1.196e-07, 1.498e-07, 1.904e-07,
  2.422e-07, 3.055e-07, 3.804e-07, 4.747e-07, 5.899e-07, 7.272e-07,
  8.91e-07, 1.071e-06, 1.296e-06, 1.546e-06, 1.823e-06, 2.135e-06,
  2.44e-06, 2.714e-06, 2.967e-06, 3.189e-06, 3.391e-06, 3.58e-06,
  3.773e-06, 4.022e-06, 4.346e-06, 4.749e-06, 5.199e-06, 5.668e-06,
  6.157e-06, 6.688e-06, 7.254e-06, 7.867e-06, 8.539e-06, 9.26e-06,
  1.009e-05, 1.119e-05, 1.228e-05, 1.365e-05, 1.506e-05, 1.641e-05,
  1.784e-05, 1.952e-05, 2.132e-05, 2.323e-05, 2.531e-05, 2.754e-05,
  3.047e-05, 3.459e-05, 3.922e-05, 4.439e-05, 4.825e-05, 5.077e-05,
  5.34e-05, 5.618e-05, 5.909e-05, 6.207e-05, 6.519e-05, 6.845e-05,
  6.819e-05, 6.726e-05, 6.622e-05, 6.512e-05, 6.671e-05, 6.862e-05,
  7.048e-05, 7.264e-05, 7.3e-05, 7.3e-05, 7.3e-05, 7.3e-05, 7.3e-05
};

static double cof2[121] = {
  7.5e-14, 1.055e-13, 1.485e-13, 2.111e-13, 3.001e-13, 4.333e-13,
  6.269e-13, 9.221e-13, 1.364e-12, 2.046e-12, 3.093e-12, 4.703e-12,
  7.225e-12, 1.113e-11, 1.66e-11, 2.088e-11, 2.626e-11, 3.433e-11,
  4.549e-11, 5.886e-11, 7.21e-11, 8.824e-11, 1.015e-10, 1.155e-10,
  1.288e-10, 1.388e-10, 1.497e-10, 1.554e-10, 1.606e-10, 1.639e-10,
  1.64e-10, 1.64e-10, 1.596e-10, 1.542e-10, 1.482e-10, 1.382e-10,
  1.289e-10, 1.198e-10, 1.109e-10, 1.026e-10, 9.484e-11, 8.75e-11,
  8.086e-11, 7.49e-11, 6.948e-11, 6.446e-11, 5.961e-11, 5.505e-11,
  5.085e-11, 4.586e-11, 4.1e-11, 3.665e-11, 3.235e-11, 2.842e-11,
  2.491e-11, 2.11e-11, 1.769e-11, 1.479e-11, 1.197e-11, 9.631e-12,
  7.74e-12, 6.201e-12, 4.963e-12, 3.956e-12, 3.151e-12, 2.507e-12,
  1.99e-12, 1.576e-12, 1.245e-12, 9.83e-13, 7.742e-13, 6.088e-13,
  4.782e-13, 3.745e-13, 2.929e-13, 2.286e-13, 1.782e-13, 1.388e-13,
  1.079e-13, 8.362e-14, 6.471e-14, 4.996e-14, 3.85e-14, 2.96e-14,
  2.265e-14, 1.729e-14, 1.317e-14, 9.998e-15, 7.549e-15, 5.683e-15,
  4.273e-15, 3.193e-15, 2.385e-15, 1.782e-15, 1.331e-15, 9.957e-16,
```

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  7.461e-16, 5.601e-16, 4.228e-16, 3.201e-16, 2.438e-16, 1.878e-16,
  1.445e-16, 1.111e-16, 8.544e-17, 6.734e-17, 5.341e-17, 4.237e-17,
  3.394e-17, 2.759e-17, 2.254e-17, 1.851e-17, 1.54e-17, 1.297e-17,
  1.096e-17, 9.365e-18, 8e-18, 6.938e-18, 6.056e-18, 5.287e-18,
  4.662e-18
};

static double f11[121] = {
  2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10,
  2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.635e-10, 2.536e-10,
  2.44e-10, 2.348e-10, 2.258e-10, 2.153e-10, 2.046e-10, 1.929e-10,
  1.782e-10, 1.648e-10, 1.463e-10, 1.291e-10, 1.1e-10, 8.874e-11,
  7.165e-11, 5.201e-11, 3.744e-11, 2.577e-11, 1.64e-11, 1.048e-11,
  5.993e-12, 3.345e-12, 1.839e-12, 9.264e-13, 4.688e-13, 2.329e-13,
  1.129e-13, 5.505e-14, 2.825e-14, 1.492e-14, 7.997e-15, 5.384e-15,
  3.988e-15, 2.955e-15, 2.196e-15, 1.632e-15, 1.214e-15, 9.025e-16,
  6.708e-16, 4.984e-16, 3.693e-16, 2.733e-16, 2.013e-16, 1.481e-16,
  1.087e-16, 7.945e-17, 5.782e-17, 4.195e-17, 3.038e-17, 2.19e-17,
  1.577e-17, 1.128e-17, 8.063e-18, 5.753e-18, 4.09e-18, 2.899e-18,
  2.048e-18, 1.444e-18, 1.015e-18, 7.12e-19, 4.985e-19, 3.474e-19,
  2.417e-19, 1.677e-19, 1.161e-19, 8.029e-20, 5.533e-20, 3.799e-20,
  2.602e-20, 1.776e-20, 1.209e-20, 8.202e-21, 5.522e-21, 3.707e-21,
  2.48e-21, 1.652e-21, 1.091e-21, 7.174e-22, 4.709e-22, 3.063e-22,
  1.991e-22, 1.294e-22, 8.412e-23, 5.483e-23, 3.581e-23, 2.345e-23,
  1.548e-23, 1.027e-23, 6.869e-24, 4.673e-24, 3.173e-24, 2.153e-24,
  1.461e-24, 1.028e-24, 7.302e-25, 5.188e-25, 3.739e-25, 2.753e-25,
  2.043e-25, 1.528e-25, 1.164e-25, 9.041e-26, 7.051e-26, 5.587e-26,
  4.428e-26, 3.588e-26, 2.936e-26, 2.402e-26, 1.995e-26
};

static double f12[121] = {
  5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10,
  5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.429e-10, 5.291e-10,
  5.155e-10, 5.022e-10, 4.893e-10, 4.772e-10, 4.655e-10, 4.497e-10,
  4.249e-10, 4.015e-10, 3.632e-10, 3.261e-10, 2.858e-10, 2.408e-10,
  2.03e-10, 1.685e-10, 1.4e-10, 1.163e-10, 9.65e-11, 8.02e-11, 6.705e-11,
  5.624e-11, 4.764e-11, 4.249e-11, 3.792e-11, 3.315e-11, 2.819e-11,
  2.4e-11, 1.999e-11, 1.64e-11, 1.352e-11, 1.14e-11, 9.714e-12,
  8.28e-12, 7.176e-12, 6.251e-12, 5.446e-12, 4.72e-12, 4.081e-12,
  3.528e-12, 3.08e-12, 2.699e-12, 2.359e-12, 2.111e-12, 1.901e-12,
  1.709e-12, 1.534e-12, 1.376e-12, 1.233e-12, 1.103e-12, 9.869e-13,
  8.808e-13, 7.859e-13, 7.008e-13, 6.241e-13, 5.553e-13, 4.935e-13,
  4.383e-13, 3.889e-13, 3.447e-13, 3.054e-13, 2.702e-13, 2.389e-13,
  2.11e-13, 1.862e-13, 1.643e-13, 1.448e-13, 1.274e-13, 1.121e-13,
  9.844e-14, 8.638e-14, 7.572e-14, 6.62e-14, 5.782e-14, 5.045e-14,
  4.394e-14, 3.817e-14, 3.311e-14, 2.87e-14, 2.48e-14, 2.142e-14,
  1.851e-14, 1.599e-14, 1.383e-14, 1.196e-14, 1.036e-14, 9e-15,
  7.828e-15, 6.829e-15, 5.992e-15, 5.254e-15, 4.606e-15, 4.037e-15,
  3.583e-15, 3.19e-15, 2.841e-15, 2.542e-15, 2.291e-15, 2.07e-15,
  1.875e-15, 1.71e-15, 1.57e-15, 1.442e-15, 1.333e-15, 1.232e-15,
  1.147e-15, 1.071e-15, 1.001e-15, 9.396e-16
};

static double f14[121] = {
  9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11,
  9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 8.91e-11, 8.73e-11, 8.46e-11,
  8.19e-11, 7.92e-11, 7.74e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11
};

static double f22[121] = {
  1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10,
  1.4e-10, 1.4e-10, 1.4e-10, 1.372e-10, 1.317e-10, 1.235e-10, 1.153e-10,
  1.075e-10, 1.002e-10, 9.332e-11, 8.738e-11, 8.194e-11, 7.7e-11,
  7.165e-11, 6.753e-11, 6.341e-11, 5.971e-11, 5.6e-11, 5.229e-11,
  4.859e-11, 4.488e-11, 4.118e-11, 3.83e-11, 3.568e-11, 3.308e-11,
  3.047e-11, 2.82e-11, 2.594e-11, 2.409e-11, 2.237e-11, 2.065e-11,
  1.894e-11, 1.771e-11, 1.647e-11, 1.532e-11, 1.416e-11, 1.332e-11,
  1.246e-11, 1.161e-11, 1.087e-11, 1.017e-11, 9.471e-12, 8.853e-12,
  8.235e-12, 7.741e-12, 7.247e-12, 6.836e-12, 6.506e-12, 6.176e-12,
  5.913e-12, 5.65e-12, 5.419e-12, 5.221e-12, 5.024e-12, 4.859e-12,
  4.694e-12, 4.546e-12, 4.414e-12, 4.282e-12, 4.15e-12, 4.019e-12,
  3.903e-12, 3.805e-12, 3.706e-12, 3.607e-12, 3.508e-12, 3.41e-12,
  3.31e-12, 3.212e-12, 3.129e-12, 3.047e-12, 2.964e-12, 2.882e-12,
```

```
  2.8e-12, 2.734e-12, 2.668e-12, 2.602e-12, 2.537e-12, 2.471e-12,
  2.421e-12, 2.372e-12, 2.322e-12, 2.273e-12, 2.224e-12, 2.182e-12,
  2.141e-12, 2.1e-12, 2.059e-12, 2.018e-12, 1.977e-12, 1.935e-12,
  1.894e-12, 1.853e-12, 1.812e-12, 1.77e-12, 1.73e-12, 1.688e-12,
  1.647e-12, 1.606e-12, 1.565e-12, 1.524e-12, 1.483e-12, 1.441e-12,
  1.4e-12, 1.359e-12, 1.317e-12, 1.276e-12, 1.235e-12, 1.194e-12,
  1.153e-12, 1.112e-12, 1.071e-12, 1.029e-12, 9.883e-13
};

static double h2o[121] = {
  0.01166, 0.008269, 0.005742, 0.003845, 0.00277, 0.001897, 0.001272,
  0.000827, 0.000539, 0.0003469, 0.0001579, 3.134e-05, 1.341e-05,
  6.764e-06, 4.498e-06, 3.703e-06, 3.724e-06, 3.899e-06, 4.002e-06,
  4.122e-06, 4.277e-06, 4.438e-06, 4.558e-06, 4.673e-06, 4.763e-06,
  4.809e-06, 4.856e-06, 4.936e-06, 5.021e-06, 5.114e-06, 5.222e-06,
  5.331e-06, 5.414e-06, 5.488e-06, 5.563e-06, 5.633e-06, 5.704e-06,
  5.767e-06, 5.819e-06, 5.872e-06, 5.914e-06, 5.949e-06, 5.984e-06,
  6.015e-06, 6.044e-06, 6.073e-06, 6.104e-06, 6.136e-06, 6.167e-06,
  6.189e-06, 6.208e-06, 6.226e-06, 6.212e-06, 6.185e-06, 6.158e-06,
  6.114e-06, 6.066e-06, 6.018e-06, 5.877e-06, 5.728e-06, 5.582e-06,
  5.437e-06, 5.296e-06, 5.156e-06, 5.02e-06, 4.886e-06, 4.754e-06,
  4.625e-06, 4.498e-06, 4.374e-06, 4.242e-06, 4.096e-06, 3.955e-06,
  3.817e-06, 3.683e-06, 3.491e-06, 3.204e-06, 2.94e-06, 2.696e-06,
  2.47e-06, 2.252e-06, 2.019e-06, 1.808e-06, 1.618e-06, 1.445e-06,
  1.285e-06, 1.105e-06, 9.489e-07, 8.121e-07, 6.938e-07, 5.924e-07,
  5.04e-07, 4.288e-07, 3.648e-07, 3.103e-07, 2.642e-07, 2.252e-07,
  1.921e-07, 1.643e-07, 1.408e-07, 1.211e-07, 1.048e-07, 9.063e-08,
  7.835e-08, 6.774e-08, 5.936e-08, 5.221e-08, 4.592e-08, 4.061e-08,
  3.62e-08, 3.236e-08, 2.902e-08, 2.62e-08, 2.383e-08, 2.171e-08,
  1.989e-08, 1.823e-08, 1.684e-08, 1.562e-08, 1.449e-08, 1.351e-08
};

static double h2o2[121] = {
  1.779e-10, 7.938e-10, 8.953e-10, 8.032e-10, 6.564e-10, 5.159e-10,
  4.003e-10, 3.026e-10, 2.222e-10, 1.58e-10, 1.044e-10, 6.605e-11,
  3.413e-11, 1.453e-11, 1.062e-11, 1.009e-11, 9.597e-12, 1.175e-11,
  1.572e-11, 2.091e-11, 2.746e-11, 3.603e-11, 4.791e-11, 6.387e-11,
  8.239e-11, 1.007e-10, 1.23e-10, 1.363e-10, 1.489e-10, 1.585e-10,
  1.608e-10, 1.632e-10, 1.576e-10, 1.502e-10, 1.423e-10, 1.302e-10,
  1.192e-10, 1.085e-10, 9.795e-11, 8.854e-11, 8.057e-11, 7.36e-11,
  6.736e-11, 6.362e-11, 6.087e-11, 5.825e-11, 5.623e-11, 5.443e-11,
  5.27e-11, 5.098e-11, 4.931e-11, 4.769e-11, 4.611e-11, 4.458e-11,
  4.308e-11, 4.102e-11, 3.887e-11, 3.682e-11, 3.521e-11, 3.369e-11,
  3.224e-11, 3.082e-11, 2.946e-11, 2.814e-11, 2.687e-11, 2.566e-11,
  2.449e-11, 2.336e-11, 2.227e-11, 2.123e-11, 2.023e-11, 1.927e-11,
  1.835e-11, 1.746e-11, 1.661e-11, 1.58e-11, 1.502e-11, 1.428e-11,
  1.357e-11, 1.289e-11, 1.224e-11, 1.161e-11, 1.102e-11, 1.045e-11,
  9.895e-12, 9.369e-12, 8.866e-12, 8.386e-12, 7.922e-12, 7.479e-12,
  7.06e-12, 6.656e-12, 6.274e-12, 5.914e-12, 5.575e-12, 5.257e-12,
  4.959e-12, 4.679e-12, 4.42e-12, 4.178e-12, 3.954e-12, 3.75e-12,
  3.557e-12, 3.372e-12, 3.198e-12, 3.047e-12, 2.908e-12, 2.775e-12,
  2.653e-12, 2.544e-12, 2.442e-12, 2.346e-12, 2.26e-12, 2.183e-12,
  2.11e-12, 2.044e-12, 1.98e-12, 1.924e-12, 1.871e-12, 1.821e-12,
  1.775e-12
};

static double hcn[121] = {
  5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10,
  5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.498e-10, 5.495e-10, 5.493e-10,
  5.49e-10, 5.488e-10, 4.717e-10, 3.946e-10, 3.174e-10, 2.4e-10,
  1.626e-10, 1.619e-10, 1.612e-10, 1.602e-10, 1.593e-10, 1.582e-10,
  1.572e-10, 1.56e-10, 1.549e-10, 1.539e-10, 1.53e-10, 1.519e-10,
  1.506e-10, 1.487e-10, 1.467e-10, 1.449e-10, 1.43e-10, 1.413e-10,
  1.397e-10, 1.382e-10, 1.368e-10, 1.354e-10, 1.337e-10, 1.315e-10,
  1.292e-10, 1.267e-10, 1.241e-10, 1.215e-10, 1.19e-10, 1.165e-10,
  1.141e-10, 1.118e-10, 1.096e-10, 1.072e-10, 1.047e-10, 1.021e-10,
  9.968e-11, 9.739e-11, 9.539e-11, 9.339e-11, 9.135e-11, 8.898e-11,
  8.664e-11, 8.439e-11, 8.249e-11, 8.075e-11, 7.904e-11, 7.735e-11,
  7.565e-11, 7.399e-11, 7.245e-11, 7.109e-11, 6.982e-11, 6.863e-11,
  6.755e-11, 6.657e-11, 6.587e-11, 6.527e-11, 6.476e-11, 6.428e-11,
  6.382e-11, 6.343e-11, 6.307e-11, 6.272e-11, 6.238e-11, 6.205e-11,
  6.17e-11, 6.137e-11, 6.102e-11, 6.072e-11, 6.046e-11, 6.03e-11,
  6.018e-11, 6.01e-11, 6.001e-11, 5.992e-11, 5.984e-11, 5.975e-11,
  5.967e-11, 5.958e-11, 5.95e-11, 5.941e-11, 5.933e-11, 5.925e-11,
  5.916e-11, 5.908e-11, 5.899e-11, 5.891e-11, 5.883e-11, 5.874e-11,
  5.866e-11, 5.858e-11, 5.85e-11, 5.841e-11, 5.833e-11, 5.825e-11,
  5.817e-11, 5.808e-11, 5.8e-11, 5.792e-11, 5.784e-11
};

static double hno3[121] = {
  1.809e-10, 7.234e-10, 5.899e-10, 4.342e-10, 3.277e-10, 2.661e-10,
  2.35e-10, 2.267e-10, 2.389e-10, 2.651e-10, 3.255e-10, 4.099e-10,
  5.42e-10, 6.978e-10, 8.807e-10, 1.112e-09, 1.405e-09, 2.04e-09,
  3.111e-09, 4.5e-09, 5.762e-09, 7.37e-09, 7.852e-09, 8.109e-09,
  8.067e-09, 7.554e-09, 7.076e-09, 6.268e-09, 5.524e-09, 4.749e-09,
  3.909e-09, 3.223e-09, 2.517e-09, 1.942e-09, 1.493e-09, 1.122e-09,
  8.449e-10, 6.361e-10, 4.787e-10, 3.611e-10, 2.804e-10, 2.215e-10,
```

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  1.758e-10, 1.441e-10, 1.197e-10, 9.953e-11, 8.505e-11, 7.334e-11,
  6.325e-11, 5.625e-11, 5.058e-11, 4.548e-11, 4.122e-11, 3.748e-11,
  3.402e-11, 3.088e-11, 2.8e-11, 2.536e-11, 2.293e-11, 2.072e-11,
  1.871e-11, 1.687e-11, 1.52e-11, 1.368e-11, 1.23e-11, 1.105e-11,
  9.922e-12, 8.898e-12, 7.972e-12, 7.139e-12, 6.385e-12, 5.708e-12,
  5.099e-12, 4.549e-12, 4.056e-12, 3.613e-12, 3.216e-12, 2.862e-12,
  2.544e-12, 2.259e-12, 2.004e-12, 1.776e-12, 1.572e-12, 1.391e-12,
  1.227e-12, 1.082e-12, 9.528e-13, 8.379e-13, 7.349e-13, 6.436e-13,
  5.634e-13, 4.917e-13, 4.291e-13, 3.745e-13, 3.267e-13, 2.854e-13,
  2.494e-13, 2.181e-13, 1.913e-13, 1.68e-13, 1.479e-13, 1.31e-13,
  1.159e-13, 1.025e-13, 9.067e-14, 8.113e-14, 7.281e-14, 6.535e-14,
  5.892e-14, 5.348e-14, 4.867e-14, 4.439e-14, 4.073e-14, 3.76e-14,
  3.476e-14, 3.229e-14, 3e-14, 2.807e-14, 2.635e-14, 2.473e-14,
  2.332e-14
};

static double hno4[121] = {
  6.118e-12, 3.594e-12, 2.807e-12, 3.04e-12, 4.458e-12, 7.986e-12,
  1.509e-11, 2.661e-11, 3.738e-11, 4.652e-11, 4.429e-11, 3.992e-11,
  3.347e-11, 3.005e-11, 3.173e-11, 4.055e-11, 5.812e-11, 8.489e-11,
  1.19e-10, 1.482e-10, 1.766e-10, 2.103e-10, 2.35e-10, 2.598e-10,
  2.801e-10, 2.899e-10, 3e-10, 2.817e-10, 2.617e-10, 2.332e-10,
  1.933e-10, 1.605e-10, 1.232e-10, 9.285e-11, 6.941e-11, 4.951e-11,
  3.539e-11, 2.402e-11, 1.522e-11, 9.676e-12, 6.056e-12, 3.745e-12,
  2.34e-12, 1.463e-12, 9.186e-13, 5.769e-13, 3.322e-13, 1.853e-13,
  1.035e-13, 7.173e-14, 5.382e-14, 4.036e-14, 3.401e-14, 2.997e-14,
  2.635e-14, 2.316e-14, 2.034e-14, 1.783e-14, 1.56e-14, 1.363e-14,
  1.19e-14, 1.037e-14, 9.032e-15, 7.846e-15, 6.813e-15, 5.912e-15,
  5.121e-15, 4.431e-15, 3.829e-15, 3.306e-15, 2.851e-15, 2.456e-15,
  2.114e-15, 1.816e-15, 1.559e-15, 1.337e-15, 1.146e-15, 9.811e-16,
  8.389e-16, 7.162e-16, 6.109e-16, 5.203e-16, 4.425e-16, 3.76e-16,
  3.184e-16, 2.692e-16, 2.274e-16, 1.917e-16, 1.61e-16, 1.35e-16,
  1.131e-16, 9.437e-17, 7.874e-17, 6.57e-17, 5.481e-17, 4.579e-17,
  3.828e-17, 3.204e-17, 2.691e-17, 2.264e-17, 1.912e-17, 1.626e-17,
  1.382e-17, 1.174e-17, 9.972e-18, 8.603e-18, 7.45e-18, 6.453e-18,
  5.623e-18, 4.944e-18, 4.361e-18, 3.859e-18, 3.443e-18, 3.096e-18,
  2.788e-18, 2.528e-18, 2.293e-18, 2.099e-18, 1.929e-18, 1.773e-18,
  1.64e-18
};

static double hocl[121] = {
  1.056e-12, 1.194e-12, 1.35e-12, 1.531e-12, 1.737e-12, 1.982e-12,
  2.263e-12, 2.599e-12, 2.991e-12, 3.459e-12, 4.012e-12, 4.662e-12,
  5.438e-12, 6.35e-12, 7.425e-12, 8.686e-12, 1.016e-11, 1.188e-11,
  1.389e-11, 1.659e-11, 2.087e-11, 2.621e-11, 3.265e-11, 4.064e-11,
  4.859e-11, 5.441e-11, 6.09e-11, 6.373e-11, 6.611e-11, 6.94e-11,
  7.44e-11, 7.97e-11, 8.775e-11, 9.722e-11, 1.064e-10, 1.089e-10,
  1.114e-10, 1.106e-10, 1.053e-10, 1.004e-10, 9.006e-11, 7.778e-11,
  6.739e-11, 5.636e-11, 4.655e-11, 3.845e-11, 3.042e-11, 2.368e-11,
  1.845e-11, 1.442e-11, 1.127e-11, 8.814e-12, 6.544e-12, 4.763e-12,
  3.449e-12, 2.612e-12, 1.999e-12, 1.526e-12, 1.16e-12, 8.793e-13,
  6.655e-13, 5.017e-13, 3.778e-13, 2.829e-13, 2.117e-13, 1.582e-13,
  1.178e-13, 8.755e-14, 6.486e-14, 4.799e-14, 3.54e-14, 2.606e-14,
  1.916e-14, 1.403e-14, 1.026e-14, 7.48e-15, 5.446e-15, 3.961e-15,
  2.872e-15, 2.076e-15, 1.498e-15, 1.077e-15, 7.726e-16, 5.528e-16,
  3.929e-16, 2.785e-16, 1.969e-16, 1.386e-16, 9.69e-17, 6.747e-17,
  4.692e-17, 3.236e-17, 2.232e-17, 1.539e-17, 1.061e-17, 7.332e-18,
  5.076e-18, 3.522e-18, 2.461e-18, 1.726e-18, 1.22e-18, 8.75e-19,
  6.264e-19, 4.482e-19, 3.207e-19, 2.368e-19, 1.762e-19, 1.312e-19,
  9.891e-20, 7.595e-20, 5.87e-20, 4.567e-20, 3.612e-20, 2.904e-20,
  2.343e-20, 1.917e-20, 1.568e-20, 1.308e-20, 1.1e-20, 9.25e-21,
  7.881e-21
};

static double n2o[121] = {
  3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07,
  3.17e-07, 3.17e-07, 3.17e-07, 3.124e-07, 3.077e-07, 3.03e-07,
  2.984e-07, 2.938e-07, 2.892e-07, 2.847e-07, 2.779e-07, 2.705e-07,
  2.631e-07, 2.557e-07, 2.484e-07, 2.345e-07, 2.201e-07, 2.01e-07,
  1.754e-07, 1.532e-07, 1.329e-07, 1.154e-07, 1.003e-07, 8.735e-08,
  7.617e-08, 6.512e-08, 5.547e-08, 4.709e-08, 3.915e-08, 3.259e-08,
  2.738e-08, 2.327e-08, 1.98e-08, 1.711e-08, 1.493e-08, 1.306e-08,
  1.165e-08, 1.049e-08, 9.439e-09, 8.375e-09, 7.391e-09, 6.525e-09,
  5.759e-09, 5.083e-09, 4.485e-09, 3.953e-09, 3.601e-09, 3.27e-09,
  2.975e-09, 2.757e-09, 2.556e-09, 2.37e-09, 2.195e-09, 2.032e-09,
  1.912e-09, 1.79e-09, 1.679e-09, 1.572e-09, 1.482e-09, 1.402e-09,
  1.326e-09, 1.254e-09, 1.187e-09, 1.127e-09, 1.071e-09, 1.02e-09,
  9.673e-10, 9.193e-10, 8.752e-10, 8.379e-10, 8.017e-10, 7.66e-10,
  7.319e-10, 7.004e-10, 6.721e-10, 6.459e-10, 6.199e-10, 5.942e-10,
  5.703e-10, 5.488e-10, 5.283e-10, 5.082e-10, 4.877e-10, 4.696e-10,
  4.52e-10, 4.355e-10, 4.198e-10, 4.039e-10, 3.888e-10, 3.754e-10,
  3.624e-10, 3.499e-10, 3.381e-10, 3.267e-10, 3.163e-10, 3.058e-10,
  2.959e-10, 2.864e-10, 2.77e-10, 2.686e-10, 2.604e-10, 2.534e-10,
  2.462e-10, 2.386e-10, 2.318e-10, 2.247e-10, 2.189e-10, 2.133e-10,
  2.071e-10, 2.014e-10, 1.955e-10, 1.908e-10, 1.86e-10, 1.817e-10
};
```

```
static double n2o5[121] = {
  1.231e-11, 3.035e-12, 1.702e-12, 9.877e-13, 8.081e-13, 9.039e-13,
  1.169e-12, 1.474e-12, 1.651e-12, 1.795e-12, 1.998e-12, 2.543e-12,
  4.398e-12, 7.698e-12, 1.28e-11, 2.131e-11, 3.548e-11, 5.894e-11,
  7.645e-11, 1.089e-10, 1.391e-10, 1.886e-10, 2.386e-10, 2.986e-10,
  3.487e-10, 3.994e-10, 4.5e-10, 4.6e-10, 4.591e-10, 4.1e-10, 3.488e-10,
  2.846e-10, 2.287e-10, 1.696e-10, 1.011e-10, 6.428e-11, 4.324e-11,
  2.225e-11, 6.214e-12, 3.608e-12, 8.793e-13, 4.491e-13, 1.04e-13,
  6.1e-14, 3.436e-14, 6.671e-15, 1.171e-15, 5.848e-16, 1.212e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16
};

static double nh3[121] = {
  1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10,
  1e-10, 1e-10, 1e-10, 1e-10, 9.444e-11, 8.488e-11, 7.241e-11, 5.785e-11,
  4.178e-11, 3.018e-11, 2.18e-11, 1.574e-11, 1.137e-11, 8.211e-12,
  5.973e-12, 4.327e-12, 3.118e-12, 2.234e-12, 1.573e-12, 1.04e-12,
  6.762e-13, 4.202e-13, 2.406e-13, 1.335e-13, 6.938e-14, 3.105e-14,
  1.609e-14, 1.033e-14, 6.432e-15, 4.031e-15, 2.555e-15, 1.656e-15,
  1.115e-15, 7.904e-16, 5.63e-16, 4.048e-16, 2.876e-16, 2.004e-16,
  1.356e-16, 9.237e-17, 6.235e-17, 4.223e-17, 3.009e-17, 2.328e-17,
  2.002e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17
};

static double no[121] = {
  2.586e-10, 4.143e-11, 1.566e-11, 9.591e-12, 8.088e-12, 8.462e-12,
  1.013e-11, 1.328e-11, 1.855e-11, 2.678e-11, 3.926e-11, 5.464e-11,
  7.012e-11, 8.912e-11, 1.127e-10, 1.347e-10, 1.498e-10, 1.544e-10,
  1.602e-10, 1.824e-10, 2.078e-10, 2.366e-10, 2.691e-10, 5.141e-10,
  8.259e-10, 1.254e-09, 1.849e-09, 2.473e-09, 3.294e-09, 4.16e-09,
  5.095e-09, 6.11e-09, 6.93e-09, 7.888e-09, 8.903e-09, 9.713e-09,
  1.052e-08, 1.115e-08, 1.173e-08, 1.21e-08, 1.228e-08, 1.239e-08,
  1.231e-08, 1.213e-08, 1.192e-08, 1.138e-08, 1.085e-08, 1.008e-08,
  9.224e-09, 8.389e-09, 7.262e-09, 6.278e-09, 5.335e-09, 4.388e-09,
  3.589e-09, 2.761e-09, 2.129e-09, 1.633e-09, 1.243e-09, 9.681e-10,
  8.355e-10, 7.665e-10, 7.442e-10, 8.584e-10, 9.732e-10, 1.063e-09,
  1.163e-09, 1.286e-09, 1.472e-09, 1.707e-09, 2.032e-09, 2.474e-09,
  2.977e-09, 3.506e-09, 4.102e-09, 5.013e-09, 6.493e-09, 8.414e-09,
  1.077e-08, 1.367e-08, 1.777e-08, 2.625e-08, 3.926e-08, 5.545e-08,
  7.195e-08, 9.464e-08, 1.404e-07, 2.183e-07, 3.329e-07, 4.535e-07,
  6.158e-07, 8.187e-07, 1.075e-06, 1.422e-06, 1.979e-06, 2.71e-06,
  3.58e-06, 4.573e-06, 5.951e-06, 7.999e-06, 1.072e-05, 1.372e-05,
  1.697e-05, 2.112e-05, 2.643e-05, 3.288e-05, 3.994e-05, 4.794e-05,
  5.606e-05, 6.383e-05, 7.286e-05, 8.156e-05, 8.883e-05, 9.469e-05,
  9.848e-05, 0.0001023, 0.0001066, 0.0001115, 0.0001145, 0.0001142,
  0.0001133
};

static double no2[121] = {
  3.036e-09, 2.945e-10, 9.982e-11, 5.069e-11, 3.485e-11, 2.982e-11,
  2.947e-11, 3.164e-11, 3.714e-11, 4.586e-11, 6.164e-11, 8.041e-11,
  9.982e-11, 1.283e-10, 1.73e-10, 2.56e-10, 3.909e-10, 5.959e-10,
  9.081e-10, 1.384e-09, 1.788e-09, 2.189e-09, 2.686e-09, 3.091e-09,
  3.49e-09, 3.796e-09, 4.2e-09, 5.103e-09, 6.005e-09, 6.3e-09, 6.706e-09,
  7.07e-09, 7.434e-09, 7.663e-09, 7.788e-09, 7.8e-09, 7.597e-09,
  7.482e-09, 7.227e-09, 6.403e-09, 5.585e-09, 4.606e-09, 3.703e-09,
  2.984e-09, 2.183e-09, 1.48e-09, 8.441e-10, 5.994e-10, 3.799e-10,
  2.751e-10, 1.927e-10, 1.507e-10, 1.102e-10, 6.971e-11, 5.839e-11,
  3.904e-11, 3.087e-11, 2.176e-11, 1.464e-11, 1.209e-11, 8.497e-12,
  6.477e-12, 4.371e-12, 2.914e-12, 2.424e-12, 1.753e-12, 1.35e-12,
  9.417e-13, 6.622e-13, 5.148e-13, 3.841e-13, 3.446e-13, 3.01e-13,
  2.551e-13, 2.151e-13, 1.829e-13, 1.64e-13, 1.475e-13, 1.352e-13,
  1.155e-13, 9.963e-14, 9.771e-14, 9.577e-14, 9.384e-14, 9.186e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14
};
```

```
static double o3[121] = {
  2.218e-08, 3.394e-08, 3.869e-08, 4.219e-08, 4.501e-08, 4.778e-08,
  5.067e-08, 5.402e-08, 5.872e-08, 6.521e-08, 7.709e-08, 9.461e-08,
  1.269e-07, 1.853e-07, 2.723e-07, 3.964e-07, 5.773e-07, 8.2e-07,
  1.155e-06, 1.59e-06, 2.076e-06, 2.706e-06, 3.249e-06, 3.848e-06,
  4.459e-06, 4.986e-06, 5.573e-06, 5.958e-06, 6.328e-06, 6.661e-06,
  6.9e-06, 7.146e-06, 7.276e-06, 7.374e-06, 7.447e-06, 7.383e-06,
  7.321e-06, 7.161e-06, 6.879e-06, 6.611e-06, 6.216e-06, 5.765e-06,
  5.355e-06, 4.905e-06, 4.471e-06, 4.075e-06, 3.728e-06, 3.413e-06,
  3.125e-06, 2.856e-06, 2.607e-06, 2.379e-06, 2.17e-06, 1.978e-06,
  1.8e-06, 1.646e-06, 1.506e-06, 1.376e-06, 1.233e-06, 1.102e-06,
  9.839e-07, 8.771e-07, 7.814e-07, 6.947e-07, 6.102e-07, 5.228e-07,
  4.509e-07, 3.922e-07, 3.501e-07, 3.183e-07, 2.909e-07, 2.686e-07,
  2.476e-07, 2.284e-07, 2.109e-07, 2.003e-07, 2.013e-07, 2.022e-07,
  2.032e-07, 2.042e-07, 2.097e-07, 2.361e-07, 2.656e-07, 2.989e-07,
  3.37e-07, 3.826e-07, 4.489e-07, 5.26e-07, 6.189e-07, 7.312e-07,
  8.496e-07, 8.444e-07, 8.392e-07, 8.339e-07, 8.286e-07, 8.234e-07,
  8.181e-07, 8.129e-07, 8.077e-07, 8.026e-07, 6.918e-07, 5.176e-07,
  3.865e-07, 2.885e-07, 2.156e-07, 1.619e-07, 1.219e-07, 9.161e-08,
  6.972e-08, 5.399e-08, 3.498e-08, 2.111e-08, 1.322e-08, 8.482e-09,
  5.527e-09, 3.423e-09, 2.071e-09, 1.314e-09, 8.529e-10, 5.503e-10,
  3.665e-10
};

static double ocs[121] = {
  6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 5.997e-10,
  5.989e-10, 5.881e-10, 5.765e-10, 5.433e-10, 5.074e-10, 4.567e-10,
  4.067e-10, 3.601e-10, 3.093e-10, 2.619e-10, 2.232e-10, 1.805e-10,
  1.46e-10, 1.187e-10, 8.03e-11, 5.435e-11, 3.686e-11, 2.217e-11,
  1.341e-11, 8.756e-12, 4.511e-12, 2.37e-12, 1.264e-12, 8.28e-13,
  5.263e-13, 3.209e-13, 1.717e-13, 9.068e-14, 4.709e-14, 2.389e-14,
  1.236e-14, 1.127e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14
};

static double sf6[121] = {
  4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12,
  4.103e-12, 4.103e-12, 4.103e-12, 4.087e-12, 4.064e-12, 4.023e-12,
  3.988e-12, 3.941e-12, 3.884e-12, 3.755e-12, 3.622e-12, 3.484e-12,
  3.32e-12, 3.144e-12, 2.978e-12, 2.811e-12, 2.653e-12, 2.489e-12,
  2.332e-12, 2.199e-12, 2.089e-12, 2.013e-12, 1.953e-12, 1.898e-12,
  1.859e-12, 1.826e-12, 1.798e-12, 1.776e-12, 1.757e-12, 1.742e-12,
  1.728e-12, 1.717e-12, 1.707e-12, 1.698e-12, 1.691e-12, 1.685e-12,
  1.679e-12, 1.675e-12, 1.671e-12, 1.668e-12, 1.665e-12, 1.663e-12,
  1.661e-12, 1.659e-12, 1.658e-12, 1.657e-12, 1.656e-12, 1.655e-12,
  1.654e-12, 1.653e-12, 1.653e-12, 1.652e-12, 1.652e-12, 1.652e-12,
  1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12,
  1.651e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12
};

static double so2[121] = {
  1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10,
  1e-10, 1e-10, 9.867e-11, 9.537e-11, 9e-11, 8.404e-11, 7.799e-11,
  7.205e-11, 6.616e-11, 6.036e-11, 5.475e-11, 5.007e-11, 4.638e-11,
  4.346e-11, 4.055e-11, 3.763e-11, 3.471e-11, 3.186e-11, 2.905e-11,
  2.631e-11, 2.358e-11, 2.415e-11, 2.949e-11, 3.952e-11, 5.155e-11,
  6.76e-11, 8.741e-11, 1.099e-10, 1.278e-10, 1.414e-10, 1.512e-10,
  1.607e-10, 1.699e-10, 1.774e-10, 1.832e-10, 1.871e-10, 1.907e-10,
  1.943e-10, 1.974e-10, 1.993e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10
};
```

```
  static int ig_co2 = -999;

  double *q[NG] = { NULL };

  /* Find emitter index of CO2... */
  if (ig_co2 == -999)
    ig_co2 = find_emitter(ctl, "CO2");

  /* Identify variable... */
  for (int ig = 0; ig < ctl->ng; ig++) {
    q[ig] = NULL;
    if (strcasecmp(ctl->emitter[ig], "C2H2") == 0)
      q[ig] = c2h2;
    if (strcasecmp(ctl->emitter[ig], "C2H6") == 0)
      q[ig] = c2h6;
    if (strcasecmp(ctl->emitter[ig], "CCl4") == 0)
      q[ig] = ccl4;
    if (strcasecmp(ctl->emitter[ig], "CH4") == 0)
      q[ig] = ch4;
    if (strcasecmp(ctl->emitter[ig], "ClO") == 0)
      q[ig] = clo;
    if (strcasecmp(ctl->emitter[ig], "ClONO2") == 0)
      q[ig] = clono2;
    if (strcasecmp(ctl->emitter[ig], "CO") == 0)
      q[ig] = co;
    if (strcasecmp(ctl->emitter[ig], "COF2") == 0)
      q[ig] = cof2;
    if (strcasecmp(ctl->emitter[ig], "F11") == 0)
      q[ig] = f11;
    if (strcasecmp(ctl->emitter[ig], "F12") == 0)
      q[ig] = f12;
    if (strcasecmp(ctl->emitter[ig], "F14") == 0)
      q[ig] = f14;
    if (strcasecmp(ctl->emitter[ig], "F22") == 0)
      q[ig] = f22;
    if (strcasecmp(ctl->emitter[ig], "H2O") == 0)
      q[ig] = h2o;
    if (strcasecmp(ctl->emitter[ig], "H2O2") == 0)
      q[ig] = h2o2;
    if (strcasecmp(ctl->emitter[ig], "HCN") == 0)
      q[ig] = hcn;
    if (strcasecmp(ctl->emitter[ig], "HNO3") == 0)
      q[ig] = hno3;
    if (strcasecmp(ctl->emitter[ig], "HNO4") == 0)
      q[ig] = hno4;
    if (strcasecmp(ctl->emitter[ig], "HOCl") == 0)
      q[ig] = hocl;
    if (strcasecmp(ctl->emitter[ig], "N2O") == 0)
      q[ig] = n2o;
    if (strcasecmp(ctl->emitter[ig], "N2O5") == 0)
      q[ig] = n2o5;
    if (strcasecmp(ctl->emitter[ig], "NH3") == 0)
      q[ig] = nh3;
    if (strcasecmp(ctl->emitter[ig], "NO") == 0)
      q[ig] = no;
    if (strcasecmp(ctl->emitter[ig], "NO2") == 0)
      q[ig] = no2;
    if (strcasecmp(ctl->emitter[ig], "O3") == 0)
      q[ig] = o3;
    if (strcasecmp(ctl->emitter[ig], "OCS") == 0)
      q[ig] = ocs;
    if (strcasecmp(ctl->emitter[ig], "SF6") == 0)
      q[ig] = sf6;
    if (strcasecmp(ctl->emitter[ig], "SO2") == 0)
      q[ig] = so2;
  }

  /* Loop over atmospheric data points... */
  for (int ip = 0; ip < atm->np; ip++) {

    /* Get altitude index... */
    int iz = locate_reg(z, 121, atm->z[ip]);

    /* Interpolate pressure... */
    atm->p[ip] = EXP(z[iz], pre[iz], z[iz + 1], pre[iz + 1], atm->z[ip]);

    /* Interpolate temperature... */
    atm->t[ip] = LIN(z[iz], tem[iz], z[iz + 1], tem[iz + 1], atm->z[ip]);

    /* Interpolate trace gases... */
    for (int ig = 0; ig < ctl->ng; ig++)
      if (q[ig] != NULL)
        atm->q[ig][ip] =
          LIN(z[iz], q[ig][iz], z[iz + 1], q[ig][iz + 1], atm->z[ip]);
      else
        atm->q[ig][ip] = 0;

```

```
    /* Set CO2... */
    if (ig_co2 >= 0)
      atm->q[ig_co2][ip] =
        371.789948e-6 + 2.026214e-6 * (atm->time[ip] - 63158400.) / 31557600.;

    /* Set extinction to zero... */
    for (int iw = 0; iw < ctl->nw; iw++)
      atm->k[iw][ip] = 0;

    /* Set cloud layer... */
    atm->clz = atm->cldz = 0;
    for (int icl = 0; icl < ctl->ncl; icl++)
      atm->clk[icl] = 0;

    /* Set surface layer... */
    atm->sfz = atm->sfp = atm->sft = 0;
    for (int isf = 0; isf < ctl->nsf; isf++)
      atm->sfeps[isf] = 1;
  }
}

/*****************************************************************************/

double ctmco2(
  double nu,
  double p,
  double t,
  double u) {

  static double co2296[2001] = { 9.3388e-5, 9.7711e-5, 1.0224e-4, 1.0697e-4,
    1.1193e-4, 1.1712e-4, 1.2255e-4, 1.2824e-4, 1.3419e-4, 1.4043e-4,
    1.4695e-4, 1.5378e-4, 1.6094e-4, 1.6842e-4, 1.7626e-4, 1.8447e-4,
    1.9307e-4, 2.0207e-4, 2.1149e-4, 2.2136e-4, 2.3169e-4, 2.4251e-4,
    2.5384e-4, 2.657e-4, 2.7813e-4, 2.9114e-4, 3.0477e-4, 3.1904e-4,
    3.3399e-4, 3.4965e-4, 3.6604e-4, 3.8322e-4, 4.0121e-4, 4.2006e-4,
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    .12584
  };

  /* Get CO2 continuum absorption... */
  double xw = nu / 2 + 1;
  if (xw >= 1 && xw < 2001) {
    int iw = (int) xw;
    double dw = xw - iw;
    double ew = 1 - dw;
    double cw296 = ew * co2296[iw - 1] + dw * co2296[iw];
    double cw260 = ew * co2260[iw - 1] + dw * co2260[iw];
    double cw230 = ew * co2230[iw - 1] + dw * co2230[iw];
    double dt230 = t - 230;
```

```
    double dt260 = t - 260;
    double dt296 = t - 296;
    double ctw = dt260 * 5.050505e-4 * dt296 * cw230 - dt230 * 9.259259e-4
      * dt296 * cw260 + dt230 * 4.208754e-4 * dt260 * cw296;
    return u / NA / 1000 * p / P0 * ctw;
  } else
    return 0;
}

/*****************************************************************************/

double ctmh2o(
  double nu,
  double p,
  double t,
  double q,
  double u) {

  static double h2o296[2001] = { .17, .1695, .172, .168, .1687, .1624, .1606,
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5.493e-14, 4.288e-14, 3.427e-14, 2.787e-14, 2.296e-14, 1.909e-14,
1.598e-14, 1.344e-14, 1.135e-14, 9.616e-15, 8.169e-15, 6.957e-15,
5.938e-15, 5.08e-15, 4.353e-15, 3.738e-15, 3.217e-15, 2.773e-15,
2.397e-15, 2.077e-15, 1.805e-15, 1.575e-15, 1.382e-15, 1.221e-15,
```

```
    1.09e-15, 9.855e-16, 9.068e-16, 8.537e-16, 8.27e-16, 8.29e-16,
    8.634e-16, 9.359e-16, 1.055e-15, 1.233e-15, 1.486e-15, 1.839e-15,
    2.326e-15, 2.998e-15, 3.934e-15, 5.256e-15, 7.164e-15, 9.984e-15,
    1.427e-14, 2.099e-14, 3.196e-14, 5.121e-14, 7.908e-14, 1.131e-13,
    1.602e-13, 2.239e-13, 3.075e-13, 4.134e-13, 5.749e-13, 7.886e-13,
    1.071e-12, 1.464e-12, 2.032e-12, 2.8e-12, 3.732e-12, 4.996e-12,
    6.483e-12, 8.143e-12, 1.006e-11, 1.238e-11, 1.484e-11, 1.744e-11,
    2.02e-11, 2.274e-11, 2.562e-11, 2.848e-11, 3.191e-11, 3.617e-11,
    4.081e-11, 4.577e-11, 4.937e-11, 5.204e-11, 5.401e-11, 5.462e-11,
    5.507e-11, 5.51e-11, 5.605e-11, 5.686e-11, 5.739e-11, 5.766e-11,
    5.74e-11, 5.754e-11, 5.761e-11, 5.777e-11, 5.712e-11, 5.51e-11,
    5.088e-11, 4.438e-11, 3.728e-11, 2.994e-11, 2.305e-11, 1.715e-11,
    1.256e-11, 9.208e-12, 6.745e-12, 5.014e-12, 3.785e-12, 2.9e-12,
    2.239e-12, 1.757e-12, 1.414e-12, 1.142e-12, 9.482e-13, 8.01e-13,
    6.961e-13, 6.253e-13, 5.735e-13, 5.433e-13, 5.352e-13, 5.493e-13,
    5.706e-13, 6.068e-13, 6.531e-13, 7.109e-13, 7.767e-13, 8.59e-13,
    9.792e-13, 1.142e-12, 1.371e-12, 1.65e-12, 1.957e-12, 2.302e-12,
    2.705e-12, 3.145e-12, 3.608e-12, 4.071e-12, 4.602e-12, 5.133e-12,
    5.572e-12, 5.987e-12, 6.248e-12, 6.533e-12, 6.757e-12, 6.935e-12,
    7.224e-12, 7.422e-12, 7.538e-12, 7.547e-12, 7.495e-12, 7.543e-12,
    7.725e-12, 8.139e-12, 8.627e-12, 9.146e-12, 9.443e-12, 9.318e-12,
    8.649e-12, 7.512e-12, 6.261e-12, 4.915e-12, 3.647e-12, 2.597e-12,
    1.785e-12, 1.242e-12, 8.66e-13, 6.207e-13, 4.61e-13, 3.444e-13,
    2.634e-13, 2.1e-13, 1.725e-13, 1.455e-13, 1.237e-13, 1.085e-13,
    9.513e-14, 7.978e-14, 6.603e-14, 5.288e-14, 4.084e-14, 2.952e-14,
    2.157e-14, 1.593e-14, 1.199e-14, 9.267e-15, 7.365e-15, 6.004e-15,
    4.995e-15, 4.218e-15, 3.601e-15, 3.101e-15, 2.692e-15, 2.36e-15,
    2.094e-15, 1.891e-15, 1.755e-15, 1.699e-15, 1.755e-15, 1.987e-15,
    2.506e-15, 3.506e-15, 5.289e-15, 8.311e-15, 1.325e-14, 2.129e-14,
    3.237e-14, 4.595e-14, 6.441e-14, 8.433e-14, 1.074e-13, 1.383e-13,
    1.762e-13, 2.281e-13, 2.831e-13, 3.523e-13, 4.38e-13, 5.304e-13,
    6.29e-13, 7.142e-13, 8.032e-13, 8.934e-13, 9.888e-13, 1.109e-12,
    1.261e-12, 1.462e-12, 1.74e-12, 2.099e-12, 2.535e-12, 3.008e-12,
    3.462e-12, 3.856e-12, 4.098e-12, 4.239e-12, 4.234e-12, 4.132e-12,
    3.986e-12, 3.866e-12, 3.829e-12, 3.742e-12, 3.705e-12, 3.694e-12,
    3.765e-12, 3.849e-12, 3.929e-12, 4.056e-12, 4.092e-12, 4.047e-12,
    3.792e-12, 3.407e-12, 2.953e-12, 2.429e-12, 1.931e-12, 1.46e-12,
    1.099e-12, 8.199e-13, 6.077e-13, 4.449e-13, 3.359e-13, 2.524e-13,
    1.881e-13, 1.391e-13, 1.02e-13, 7.544e-14, 5.555e-14, 4.22e-14,
    3.321e-14, 2.686e-14, 2.212e-14, 1.78e-14, 1.369e-14, 1.094e-14,
    9.13e-15, 8.101e-15, 7.828e-15, 8.393e-15, 1.012e-14, 1.259e-14,
    1.538e-14, 1.961e-14, 2.619e-14, 3.679e-14, 5.049e-14, 6.917e-14,
    8.88e-14, 1.115e-13, 1.373e-13, 1.619e-13, 1.878e-13, 2.111e-13,
    2.33e-13, 2.503e-13, 2.613e-13, 2.743e-13, 2.826e-13, 2.976e-13,
    3.162e-13, 3.36e-13, 3.491e-13, 3.541e-13, 3.595e-13, 3.608e-13,
    3.709e-13, 3.869e-13, 4.12e-13, 4.366e-13, 4.504e-13, 4.379e-13,
    3.955e-13, 3.385e-13, 2.741e-13, 2.089e-13, 1.427e-13, 9.294e-14,
    5.775e-14, 3.565e-14, 2.21e-14, 1.398e-14, 9.194e-15, 6.363e-15,
    4.644e-15, 3.55e-15, 2.808e-15, 2.274e-15, 1.871e-15, 1.557e-15,
    1.308e-15, 1.108e-15, 9.488e-16, 8.222e-16, 7.238e-16, 6.506e-16,
    6.008e-16, 5.742e-16, 5.724e-16, 5.991e-16, 6.625e-16, 7.775e-16,
    9.734e-16, 1.306e-15, 1.88e-15, 2.879e-15, 4.616e-15, 7.579e-15,
    1.248e-14, 2.03e-14, 3.244e-14, 5.171e-14, 7.394e-14, 9.676e-14,
    1.199e-13, 1.467e-13, 1.737e-13, 2.02e-13, 2.425e-13, 3.016e-13,
    3.7e-13, 4.617e-13, 5.949e-13, 7.473e-13, 9.378e-13, 1.191e-12,
    1.481e-12, 1.813e-12, 2.232e-12, 2.722e-12, 3.254e-12, 3.845e-12,
    4.458e-12, 5.048e-12, 5.511e-12, 5.898e-12, 6.204e-12, 6.293e-12,
    6.386e-12, 6.467e-12, 6.507e-12, 6.466e-12, 6.443e-12, 6.598e-12,
    6.873e-12, 7.3e-12, 7.816e-12, 8.368e-12, 8.643e-12, 8.466e-12,
    7.871e-12, 6.853e-12, 5.714e-12, 4.482e-12, 3.392e-12, 2.613e-12,
    2.008e-12, 1.562e-12, 1.228e-12, 9.888e-13, 7.646e-13, 5.769e-13,
    4.368e-13, 3.324e-13, 2.508e-13, 1.916e-13
  };

  static double xfcrev[15] =
    { 1.003, 1.009, 1.015, 1.023, 1.029, 1.033, 1.037,
    1.039, 1.04, 1.046, 1.036, 1.027, 1.01, 1.002, 1.
  };

  double sfac;

  /* Get H2O continuum absorption... */
  double xw = nu / 10 + 1;
  if (xw >= 1 && xw < 2001) {
    int iw = (int) xw;
    double dw = xw - iw;
    double ew = 1 - dw;
    double cw296 = ew * h2o296[iw - 1] + dw * h2o296[iw];
    double cw260 = ew * h2o260[iw - 1] + dw * h2o260[iw];
    double cwfrn = ew * h2ofrn[iw - 1] + dw * h2ofrn[iw];
    if (nu <= 820 || nu >= 960) {
      sfac = 1;
    } else {
      double xx = (nu - 820) / 10;
      int ix = (int) xx;
      double dx = xx - ix;
      sfac = (1 - dx) * xfcrev[ix] + dx * xfcrev[ix + 1];
```

```
    }
    double ctwslf =
      sfac * cw296 * pow(cw260 / cw296, (296 - t) / (296 - 260));
    double vf2 = POW2(nu - 370);
    double vf6 = POW3(vf2);
    double fscal = 36100 / (vf2 + vf6 * 1e-8 + 36100) * -.25 + 1;
    double ctwfrn = cwfrn * fscal;
    double a1 = nu * u * tanh(.7193876 / t * nu);
    double a2 = 296 / t;
    double a3 = p / P0 * (q * ctwslf + (1 - q) * ctwfrn) * 1e-20;
    return a1 * a2 * a3;
  } else
    return 0;
}

/*****************************************************************************/

double ctmn2(
  double nu,
  double p,
  double t) {

  static double ba[98] = { 0., 4.45e-8, 5.22e-8, 6.46e-8, 7.75e-8, 9.03e-8,
    1.06e-7, 1.21e-7, 1.37e-7, 1.57e-7, 1.75e-7, 2.01e-7, 2.3e-7,
    2.59e-7, 2.95e-7, 3.26e-7, 3.66e-7, 4.05e-7, 4.47e-7, 4.92e-7,
    5.34e-7, 5.84e-7, 6.24e-7, 6.67e-7, 7.14e-7, 7.26e-7, 7.54e-7,
    7.84e-7, 8.09e-7, 8.42e-7, 8.62e-7, 8.87e-7, 9.11e-7, 9.36e-7,
    9.76e-7, 1.03e-6, 1.11e-6, 1.23e-6, 1.39e-6, 1.61e-6, 1.76e-6,
    1.94e-6, 1.97e-6, 1.87e-6, 1.75e-6, 1.56e-6, 1.42e-6, 1.35e-6,
    1.32e-6, 1.29e-6, 1.29e-6, 1.3e-6, 1.32e-6, 1.33e-6,
    1.34e-6, 1.35e-6, 1.33e-6, 1.31e-6, 1.29e-6, 1.24e-6, 1.2e-6,
    1.16e-6, 1.1e-6, 1.04e-6, 9.96e-7, 9.38e-7, 8.63e-7, 7.98e-7,
    7.26e-7, 6.55e-7, 5.94e-7, 5.35e-7, 4.74e-7, 4.24e-7, 3.77e-7,
    3.33e-7, 2.96e-7, 2.63e-7, 2.34e-7, 2.08e-7, 1.85e-7, 1.67e-7,
    1.47e-7, 1.32e-7, 1.2e-7, 1.09e-7, 9.85e-8, 9.08e-8, 8.18e-8,
    7.56e-8, 6.85e-8, 6.14e-8, 5.83e-8, 5.77e-8, 5e-8, 4.32e-8, 0.
  };

  static double betaa[98] = { 802., 802., 761., 722., 679., 646., 609., 562.,
    511., 472., 436., 406., 377., 355., 338., 319., 299., 278., 255.,
    233., 208., 184., 149., 107., 66., 25., -13., -49., -82., -104.,
    -119., -130., -139., -144., -146., -146., -147., -148., -150.,
    -153., -160., -169., -181., -189., -195., -200., -205., -209.,
    -211., -210., -210., -209., -205., -199., -190., -180., -168.,
    -157., -143., -126., -108., -89., -63., -32., 1., 35., 65., 95.,
    121., 141., 152., 161., 164., 164., 161., 155., 148., 143., 137.,
    133., 131., 133., 139., 150., 165., 187., 213., 248., 284., 321.,
    372., 449., 514., 569., 609., 642., 673., 673.
  };

  static double nua[98] = { 2120., 2125., 2130., 2135., 2140., 2145., 2150.,
    2155., 2160., 2165., 2170., 2175., 2180., 2185., 2190., 2195.,
    2200., 2205., 2210., 2215., 2220., 2225., 2230., 2235., 2240.,
    2245., 2250., 2255., 2260., 2265., 2270., 2275., 2280., 2285.,
    2290., 2295., 2300., 2305., 2310., 2315., 2320., 2325., 2330.,
    2335., 2340., 2345., 2350., 2355., 2360., 2365., 2370., 2375.,
    2380., 2385., 2390., 2395., 2400., 2405., 2410., 2415., 2420.,
    2425., 2430., 2435., 2440., 2445., 2450., 2455., 2460., 2465.,
    2470., 2475., 2480., 2485., 2490., 2495., 2500., 2505., 2510.,
    2515., 2520., 2525., 2530., 2535., 2540., 2545., 2550., 2555.,
    2560., 2565., 2570., 2575., 2580., 2585., 2590., 2595., 2600., 2605.
  };

  const double q_n2 = 0.79, t0 = 273.0, tr = 296.0;

  /* Check wavenumber range... */
  if (nu < nua[0] || nu > nua[97])
    return 0;

  /* Interpolate B and beta... */
  int idx = locate_reg(nua, 98, nu);
  double b = LIN(nua[idx], ba[idx], nua[idx + 1], ba[idx + 1], nu);
  double beta = LIN(nua[idx], betaa[idx], nua[idx + 1], betaa[idx + 1], nu);

  /* Compute absorption coefficient... */
  return 0.1 * POW2(p / P0 * t0 / t) * exp(beta * (1 / tr - 1 / t))
    * q_n2 * b * (q_n2 + (1 - q_n2) * (1.294 - 0.4545 * t / tr));
}

/*****************************************************************************/

double ctmo2(
  double nu,
  double p,
  double t) {

  static double ba[90] = { 0., .061, .074, .084, .096, .12, .162, .208, .246,
```

```
    .285, .314, .38, .444, .5, .571, .673, .768, .853, .966, 1.097,
    1.214, 1.333, 1.466, 1.591, 1.693, 1.796, 1.922, 2.037, 2.154,
    2.264, 2.375, 2.508, 2.671, 2.847, 3.066, 3.417, 3.828, 4.204,
    4.453, 4.599, 4.528, 4.284, 3.955, 3.678, 3.477, 3.346, 3.29,
    3.251, 3.231, 3.226, 3.212, 3.192, 3.108, 3.033, 2.911, 2.798,
    2.646, 2.508, 2.322, 2.13, 1.928, 1.757, 1.588, 1.417, 1.253,
    1.109, .99, .888, .791, .678, .587, .524, .464, .403, .357, .32,
    .29, .267, .242, .215, .182, .16, .146, .128, .103, .087, .081,
    .071, .064, 0.
  };

  static double betaa[90] = { 467., 467., 400., 315., 379., 368., 475., 521.,
    531., 512., 442., 444., 430., 381., 335., 324., 296., 248., 215.,
    193., 158., 127., 101., 71., 31., -6., -26., -47., -63., -79.,
    -88., -88., -87., -90., -98., -99., -109., -134., -160., -167.,
    -164., -158., -153., -151., -156., -166., -168., -173., -170.,
    -161., -145., -126., -108., -84., -59., -29., 4., 41., 73., 97.,
    123., 159., 198., 220., 242., 256., 281., 311., 334., 319., 313.,
    321., 323., 310., 315., 320., 335., 361., 378., 373., 338., 319.,
    346., 322., 291., 290., 350., 371., 504., 504.
  };

  static double nua[90] = { 1360., 1365., 1370., 1375., 1380., 1385., 1390.,
    1395., 1400., 1405., 1410., 1415., 1420., 1425., 1430., 1435.,
    1440., 1445., 1450., 1455., 1460., 1465., 1470., 1475., 1480.,
    1485., 1490., 1495., 1500., 1505., 1510., 1515., 1520., 1525.,
    1530., 1535., 1540., 1545., 1550., 1555., 1560., 1565., 1570.,
    1575., 1580., 1585., 1590., 1595., 1600., 1605., 1610., 1615.,
    1620., 1625., 1630., 1635., 1640., 1645., 1650., 1655., 1660.,
    1665., 1670., 1675., 1680., 1685., 1690., 1695., 1700., 1705.,
    1710., 1715., 1720., 1725., 1730., 1735., 1740., 1745., 1750.,
    1755., 1760., 1765., 1770., 1775., 1780., 1785., 1790., 1795.,
    1800., 1805.
  };

  const double q_o2 = 0.21, t0 = 273, tr = 296;

  /* Check wavenumber range... */
  if (nu < nua[0] || nu > nua[89])
    return 0;

  /* Interpolate B and beta... */
  int idx = locate_reg(nua, 90, nu);
  double b = LIN(nua[idx], ba[idx], nua[idx + 1], ba[idx + 1], nu);
  double beta = LIN(nua[idx], betaa[idx], nua[idx + 1], betaa[idx + 1], nu);

  /* Compute absorption coefficient... */
  return 0.1 * POW2(p / P0 * t0 / t) * exp(beta * (1 / tr - 1 / t)) * q_o2 *
    b;
}

/*****************************************************************************/

void copy_atm(
  ctl_t * ctl,
  atm_t * atm_dest,
  atm_t * atm_src,
  int init) {

  /* Data size... */
  size_t s = (size_t) atm_src->np * sizeof(double);

  /* Copy data... */
  atm_dest->np = atm_src->np;
  memcpy(atm_dest->time, atm_src->time, s);
  memcpy(atm_dest->z, atm_src->z, s);
  memcpy(atm_dest->lon, atm_src->lon, s);
  memcpy(atm_dest->lat, atm_src->lat, s);
  memcpy(atm_dest->p, atm_src->p, s);
  memcpy(atm_dest->t, atm_src->t, s);
  for (int ig = 0; ig < ctl->ng; ig++)
    memcpy(atm_dest->q[ig], atm_src->q[ig], s);
  for (int iw = 0; iw < ctl->nw; iw++)
    memcpy(atm_dest->k[iw], atm_src->k[iw], s);
  atm_dest->clz = atm_src->clz;
  atm_dest->cldz = atm_src->cldz;
  for (int icl = 0; icl < ctl->ncl; icl++)
    atm_dest->clk[icl] = atm_src->clk[icl];
  atm_dest->sfz = atm_src->sfz;
  atm_dest->sfp = atm_src->sfp;
  atm_dest->sft = atm_src->sft;
  for (int isf = 0; isf < ctl->nsf; isf++)
    atm_dest->sfeps[isf] = atm_src->sfeps[isf];

  /* Initialize... */
  if (init)
    for (int ip = 0; ip < atm_dest->np; ip++) {
```

```
      atm_dest->p[ip] = 0;
      atm_dest->t[ip] = 0;
      for (int ig = 0; ig < ctl->ng; ig++)
        atm_dest->q[ig][ip] = 0;
      for (int iw = 0; iw < ctl->nw; iw++)
        atm_dest->k[iw][ip] = 0;
      atm_dest->clz = 0;
      atm_dest->cldz = 0;
      for (int icl = 0; icl < ctl->ncl; icl++)
        atm_dest->clk[icl] = 0;
      atm_dest->sfz = 0;
      atm_dest->sfp = 0;
      atm_dest->sft = 0;
      for (int isf = 0; isf < ctl->nsf; isf++)
        atm_dest->sfeps[isf] = 1;
    }
}

/*****************************************************************************/

void copy_obs(
  ctl_t * ctl,
  obs_t * obs_dest,
  obs_t * obs_src,
  int init) {

  /* Data size... */
  size_t s = (size_t) obs_src->nr * sizeof(double);

  /* Copy data... */
  obs_dest->nr = obs_src->nr;
  memcpy(obs_dest->time, obs_src->time, s);
  memcpy(obs_dest->obsz, obs_src->obsz, s);
  memcpy(obs_dest->obslon, obs_src->obslon, s);
  memcpy(obs_dest->obslat, obs_src->obslat, s);
  memcpy(obs_dest->vpz, obs_src->vpz, s);
  memcpy(obs_dest->vplon, obs_src->vplon, s);
  memcpy(obs_dest->vplat, obs_src->vplat, s);
  memcpy(obs_dest->tpz, obs_src->tpz, s);
  memcpy(obs_dest->tplon, obs_src->tplon, s);
  memcpy(obs_dest->tplat, obs_src->tplat, s);
  for (int id = 0; id < ctl->nd; id++)
    memcpy(obs_dest->rad[id], obs_src->rad[id], s);
  for (int id = 0; id < ctl->nd; id++)
    memcpy(obs_dest->tau[id], obs_src->tau[id], s);

  /* Initialize... */
  if (init)
    for (int id = 0; id < ctl->nd; id++)
      for (int ir = 0; ir < obs_dest->nr; ir++)
        if (gsl_finite(obs_dest->rad[id][ir])) {
          obs_dest->rad[id][ir] = 0;
          obs_dest->tau[id][ir] = 0;
        }
}

/*****************************************************************************/

int find_emitter(
  ctl_t * ctl,
  const char *emitter) {

  for (int ig = 0; ig < ctl->ng; ig++)
    if (strcasecmp(ctl->emitter[ig], emitter) == 0)
      return ig;

  return -1;
}

/*****************************************************************************/

void formod(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs) {

  int *mask;

  /* Allocate... */
  ALLOC(mask, int,
        ND * NR);

  /* Save observation mask... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ir = 0; ir < obs->nr; ir++)
      mask[id * NR + ir] = !gsl_finite(obs->rad[id][ir]);

```

```
  /* Hydrostatic equilibrium... */
  hydrostatic(ctl, atm);

  /* EGA forward model... */
  if (ctl->formod == 1)
    for (int ir = 0; ir < obs->nr; ir++)
      formod_pencil(ctl, atm, obs, ir);

  /* Call RFM... */
  else if (ctl->formod == 2)
    formod_rfm(ctl, atm, obs);

  /* Apply field-of-view convolution... */
  formod_fov(ctl, obs);

  /* Convert radiance to brightness temperature... */
  if (ctl->write_bbt)
    for (int id = 0; id < ctl->nd; id++)
      for (int ir = 0; ir < obs->nr; ir++)
        obs->rad[id][ir] = brightness(obs->rad[id][ir], ctl->nu[id]);

  /* Apply observation mask... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ir = 0; ir < obs->nr; ir++)
      if (mask[id * NR + ir])
        obs->rad[id][ir] = GSL_NAN;

  /* Free... */
  free(mask);
}

/*****************************************************************************/

void formod_continua(
  ctl_t * ctl,
  los_t * los,
  int ip,
  double *beta) {

  static int ig_co2 = -999, ig_h2o = -999;

  /* Extinction... */
  for (int id = 0; id < ctl->nd; id++)
    beta[id] = los->k[ip][id];

  /* CO2 continuum... */
  if (ctl->ctm_co2) {
    if (ig_co2 == -999)
      ig_co2 = find_emitter(ctl, "CO2");
    if (ig_co2 >= 0)
      for (int id = 0; id < ctl->nd; id++)
        beta[id] += ctmco2(ctl->nu[id], los->p[ip], los->t[ip],
                           los->u[ip][ig_co2]) / los->ds[ip];
  }

  /* H2O continuum... */
  if (ctl->ctm_h2o) {
    if (ig_h2o == -999)
      ig_h2o = find_emitter(ctl, "H2O");
    if (ig_h2o >= 0)
      for (int id = 0; id < ctl->nd; id++)
        beta[id] += ctmh2o(ctl->nu[id], los->p[ip], los->t[ip],
                           los->q[ip][ig_h2o], los->u[ip][ig_h2o])
          / los->ds[ip];
  }

  /* N2 continuum... */
  if (ctl->ctm_n2)
    for (int id = 0; id < ctl->nd; id++)
      beta[id] += ctmn2(ctl->nu[id], los->p[ip], los->t[ip]);

  /* O2 continuum... */
  if (ctl->ctm_o2)
    for (int id = 0; id < ctl->nd; id++)
      beta[id] += ctmo2(ctl->nu[id], los->p[ip], los->t[ip]);
}

/*****************************************************************************/

void formod_fov(
  ctl_t * ctl,
  obs_t * obs) {

  static double dz[NSHAPE], w[NSHAPE];

  static int init = 0, n;

```

```
  obs_t *obs2;

  double rad[ND][NR], tau[ND][NR], z[NR];

  /* Do not take into account FOV... */
  if (ctl->fov[0] == '-')
    return;

  /* Initialize FOV data... */
  if (!init) {
    init = 1;
    read_shape(ctl->fov, dz, w, &n);
  }

  /* Allocate... */
  ALLOC(obs2, obs_t, 1);

  /* Copy observation data... */
  copy_obs(ctl, obs2, obs, 0);

  /* Loop over ray paths... */
  for (int ir = 0; ir < obs->nr; ir++) {

    /* Get radiance and transmittance profiles... */
    int nz = 0;
    for (int ir2 = GSL_MAX(ir - NFOV, 0);
         ir2 < GSL_MIN(ir + 1 + NFOV, obs->nr); ir2++)
      if (obs->time[ir2] == obs->time[ir]) {
        z[nz] = obs2->vpz[ir2];
        for (int id = 0; id < ctl->nd; id++) {
          rad[id][nz] = obs2->rad[id][ir2];
          tau[id][nz] = obs2->tau[id][ir2];
        }
        nz++;
      }
    if (nz < 2)
      ERRMSG("Cannot apply FOV convolution!");

    /* Convolute profiles with FOV... */
    double wsum = 0;
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] = 0;
      obs->tau[id][ir] = 0;
    }
    for (int i = 0; i < n; i++) {
      double zfov = obs->vpz[ir] + dz[i];
      int idx = locate_irr(z, nz, zfov);
      for (int id = 0; id < ctl->nd; id++) {
        obs->rad[id][ir] += w[i]
          * LIN(z[idx], rad[id][idx], z[idx + 1], rad[id][idx + 1], zfov);
        obs->tau[id][ir] += w[i]
          * LIN(z[idx], tau[id][idx], z[idx + 1], tau[id][idx + 1], zfov);
      }
      wsum += w[i];
    }
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] /= wsum;
      obs->tau[id][ir] /= wsum;
    }
  }

  /* Free... */
  free(obs2);
}

/*****************************************************************************/

void formod_pencil(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs,
  int ir) {

  static tbl_t *tbl;

  static int init = 0;

  los_t *los;

  double beta_ctm[ND], rad[ND], tau[ND], tau_refl[ND],
    tau_path[ND][NG], tau_gas[ND], x0[3], x1[3];

  /* Initialize look-up tables... */
  if (!init) {
    init = 1;
    ALLOC(tbl, tbl_t, 1);
    read_tbl(ctl, tbl);
```

```
    init_srcfunc(ctl, tbl);
  }

  /* Allocate... */
  ALLOC(los, los_t, 1);

  /* Initialize... */
  for (int id = 0; id < ctl->nd; id++) {
    rad[id] = 0;
    tau[id] = 1;
    for (int ig = 0; ig < ctl->ng; ig++)
      tau_path[id][ig] = 1;
  }

  /* Raytracing... */
  raytrace(ctl, atm, obs, los, ir);

  /* Loop over LOS points... */
  for (int ip = 0; ip < los->np; ip++) {

    /* Get trace gas transmittance... */
    intpol_tbl(ctl, tbl, los, ip, tau_path, tau_gas);

    /* Get continuum absorption... */
    formod_continua(ctl, los, ip, beta_ctm);

    /* Compute Planck function... */
    formod_srcfunc(ctl, tbl, los->t[ip], los->src[ip]);

    /* Loop over channels... */
    for (int id = 0; id < ctl->nd; id++)
      if (tau_gas[id] > 0) {

        /* Get segment emissivity... */
        los->eps[ip][id] = 1 - tau_gas[id] * exp(-beta_ctm[id] * los->ds[ip]);

        /* Compute radiance... */
        rad[id] += los->src[ip][id] * los->eps[ip][id] * tau[id];

        /* Compute path transmittance... */
        tau[id] *= (1 - los->eps[ip][id]);
      }
  }

  /* Check whether LOS hit the ground... */
  if (ctl->sftype >= 1 && los->sft > 0) {

    /* Add surface emissions... */
    double src_sf[ND];
    formod_srcfunc(ctl, tbl, los->sft, src_sf);
    for (int id = 0; id < ctl->nd; id++)
      rad[id] += los->sfeps[id] * src_sf[id] * tau[id];

    /* Check reflectivity... */
    int refl = 0;
    if (ctl->sftype >= 2)
      for (int id = 0; id < ctl->nd; id++)
        if (los->sfeps[id] < 1) {
          refl = 1;
          break;
        }

    /* Calculate reflection... */
    if (refl) {

      /* Initialize... */
      for (int id = 0; id < ctl->nd; id++)
        tau_refl[id] = 1;

      /* Add down-welling radiance... */
      for (int ip = los->np - 1; ip >= 0; ip--)
        for (int id = 0; id < ctl->nd; id++) {
          rad[id] += los->src[ip][id] * los->eps[ip][id] * tau_refl[id]
            * tau[id] * (1 - los->sfeps[id]);
          tau_refl[id] *= (1 - los->eps[ip][id]);
        }

      /* Add solar term... */
      if (ctl->sftype >= 3) {

        /* Get solar zenith angle... */
        double sza2;
        if (ctl->sfsza < 0)
          sza2 =
            sza(obs->time[ir], los->lon[los->np - 1], los->lat[los->np - 1]);
        else
          sza2 = ctl->sfsza;
```

```
        /* Check solar zenith angle... */
        if (sza2 < 89.999) {

          /* Get angle of incidence... */
          geo2cart(los->z[los->np - 1], los->lon[los->np - 1],
                   los->lat[los->np - 1], x0);
          geo2cart(los->z[0], los->lon[0], los->lat[0], x1);
          for (int i = 0; i < 3; i++)
            x1[i] -= x0[i];
          double cosa = DOTP(x0, x1) / NORM(x0) / NORM(x1);

          /* Get ratio of SZA and incident radiation... */
          double rcos = cosa / cos(sza2 * M_PI / 180.);

          /* Add solar radiation... */
          for (int id = 0; id < ctl->nd; id++)
            rad[id] += 6.764e-5 / (2. * M_PI) * planck(TSUN, ctl->nu[id])
              * tau_refl[id] * (1 - los->sfeps[id]) * tau[id] * rcos;
        }
      }
    }
  }

  /* Copy results... */
  for (int id = 0; id < ctl->nd; id++) {
    obs->rad[id][ir] = rad[id];
    obs->tau[id][ir] = tau[id];
  }

  /* Free... */
  free(los);
}

/*****************************************************************************/

void formod_rfm(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs) {

  los_t *los;

  FILE *out;

  char cmd[2 * LEN], filename[2 * LEN],
    rfmflg[LEN] = { "RAD TRA MIX LIN SFC" };

  double f[NSHAPE], nu[NSHAPE], nu0, nu1, obsz = -999, tsurf,
    xd[3], xo[3], xv[3], z[NR], zmin, zmax;

  int i, id, ig, ip, ir, iw, n, nadir = 0;

  /* Allocate... */
  ALLOC(los, los_t, 1);

  /* Check observer positions... */
  for (ir = 1; ir < obs->nr; ir++)
    if (obs->obsz[ir] != obs->obsz[0]
        || obs->obslon[ir] != obs->obslon[0]
        || obs->obslat[ir] != obs->obslat[0])
      ERRMSG("RFM interface requires identical observer positions!");

  /* Check extinction data... */
  for (iw = 0; iw < ctl->nw; iw++)
    for (ip = 0; ip < atm->np; ip++)
      if (atm->k[iw][ip] != 0)
        ERRMSG("RFM interface cannot handle extinction data!");

  /* Get altitude range of atmospheric data... */
  gsl_stats_minmax(&zmin, &zmax, atm->z, 1, (size_t) atm->np);

  /* Observer within atmosphere? */
  if (obs->obsz[0] >= zmin && obs->obsz[0] <= zmax) {
    obsz = obs->obsz[0];
    strcat(rfmflg, " OBS");
  }

  /* Determine tangent altitude or air mass factor... */
  for (ir = 0; ir < obs->nr; ir++) {

    /* Raytracing... */
    raytrace(ctl, atm, obs, los, ir);

    /* Nadir? */
    if (obs->tpz[ir] <= zmin) {
      geo2cart(obs->obsz[ir], obs->obslon[ir], obs->obslat[ir], xo);
```

```
      geo2cart(obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], xv);
      for (i = 0; i < 3; i++)
        xd[i] = xo[i] - xv[i];
      z[ir] = NORM(xo) * NORM(xd) / DOTP(xo, xd);
      nadir++;
    } else
      z[ir] = obs->tpz[ir];
  }
  if (nadir > 0 && nadir < obs->nr)
    ERRMSG("Limb and nadir not simultaneously possible!");

  /* Nadir? */
  if (nadir)
    strcat(rfmflg, " NAD");

  /* Get surface temperature... */
  tsurf = atm->t[gsl_stats_min_index(atm->z, 1, (size_t) atm->np)];

  /* Refraction? */
  if (!nadir && !ctl->refrac)
    strcat(rfmflg, " GEO");

  /* Continua? */
  if (ctl->ctm_co2 || ctl->ctm_h2o || ctl->ctm_n2 || ctl->ctm_o2)
    strcat(rfmflg, " CTM");

  /* Write atmospheric data file... */
  write_atm_rfm("rfm.atm", ctl, atm);

  /* Loop over channels... */
  for (id = 0; id < ctl->nd; id++) {

    /* Read filter function... */
    sprintf(filename, "%s_%.4f.filt", ctl->tblbase, ctl->nu[id]);
    read_shape(filename, nu, f, &n);

    /* Set spectral range... */
    nu0 = nu[0];
    nu1 = nu[n - 1];

    /* Create RFM driver file... */
    if (!(out = fopen("rfm.drv", "w")))
      ERRMSG("Cannot create file!");
    fprintf(out, "*HDR\nRFM call by JURASSIC.\n");
    fprintf(out, "*FLG\n%s\n", rfmflg);
    fprintf(out, "*SPC\n%.4f %.4f 0.0005\n", nu0, nu1);
    fprintf(out, "*GAS\n");
    for (ig = 0; ig < ctl->ng; ig++)
      fprintf(out, "%s\n", ctl->emitter[ig]);
    fprintf(out, "*ATM\nrfm.atm\n");
    fprintf(out, "*TAN\n");
    for (ir = 0; ir < obs->nr; ir++)
      fprintf(out, "%g\n", z[ir]);
    fprintf(out, "*SFC\n%g 1.0\n", tsurf);
    if (obsz >= 0)
      fprintf(out, "*OBS\n%g\n", obsz);
    fprintf(out, "*HIT\n%s\n", ctl->rfmhit);
    fprintf(out, "*XSC\n");
    for (ig = 0; ig < ctl->ng; ig++)
      if (ctl->rfmxsc[ig][0] != '-')
        fprintf(out, "%s\n", ctl->rfmxsc[ig]);
    fprintf(out, "*END\n");
    fclose(out);

    /* Remove temporary files... */
    if (system("rm -f rfm.runlog rad_*.asc tra_*.asc"))
      ERRMSG("Cannot remove temporary files!");

    /* Call RFM... */
    sprintf(cmd, "echo | %s", ctl->rfmbin);
    if (system(cmd))
      ERRMSG("Error while calling RFM!");

    /* Read data... */
    for (ir = 0; ir < obs->nr; ir++) {
      obs->rad[id][ir] = read_obs_rfm("rad", z[ir], nu, f, n) * 1e-5;
      obs->tau[id][ir] = read_obs_rfm("tra", z[ir], nu, f, n);
    }
  }

  /* Remove temporary files... */
  if (system("rm -f rfm.drv rfm.atm rfm.runlog rad_*.asc tra_*.asc"))
    ERRMSG("Error while removing temporary files!");

  /* Free... */
  free(los);
}
```

```
/*****************************************************************************/

void formod_srcfunc(
  ctl_t * ctl,
  tbl_t * tbl,
  double t,
  double *src) {

  /* Determine index in temperature array... */
  int it = locate_reg(tbl->st, TBLNS, t);

  /* Interpolate Planck function value... */
  for (int id = 0; id < ctl->nd; id++)
    src[id] = LIN(tbl->st[it], tbl->sr[it][id],
                  tbl->st[it + 1], tbl->sr[it + 1][id], t);
}

/*****************************************************************************/

void geo2cart(
  double z,
  double lon,
  double lat,
  double *x) {

  double radius = z + RE;

  x[0] = radius * cos(lat / 180 * M_PI) * cos(lon / 180 * M_PI);
  x[1] = radius * cos(lat / 180 * M_PI) * sin(lon / 180 * M_PI);
  x[2] = radius * sin(lat / 180 * M_PI);
}

/*****************************************************************************/

void hydrostatic(
  ctl_t * ctl,
  atm_t * atm) {

  const double mmair = 28.96456e-3, mmh2o = 18.0153e-3;

  const int ipts = 20;

  static int ig_h2o = -999;

  double dzmin = 1e99, e = 0;

  int ipref = 0;

  /* Check reference height... */
  if (ctl->hydz < 0)
    return;

  /* Determine emitter index of H2O... */
  if (ig_h2o == -999)
    ig_h2o = find_emitter(ctl, "H2O");

  /* Find air parcel next to reference height... */
  for (int ip = 0; ip < atm->np; ip++)
    if (fabs(atm->z[ip] - ctl->hydz) < dzmin) {
      dzmin = fabs(atm->z[ip] - ctl->hydz);
      ipref = ip;
    }

  /* Upper part of profile... */
  for (int ip = ipref + 1; ip < atm->np; ip++) {
    double mean = 0;
    for (int i = 0; i < ipts; i++) {
      if (ig_h2o >= 0)
        e = LIN(0.0, atm->q[ig_h2o][ip - 1],
                ipts - 1.0, atm->q[ig_h2o][ip], (double) i);
      mean += (e * mmh2o + (1 - e) * mmair)
        * G0 / RI
        / LIN(0.0, atm->t[ip - 1], ipts - 1.0, atm->t[ip], (double) i) / ipts;
    }

    /* Compute p(z,T)... */
    atm->p[ip] =
      exp(log(atm->p[ip - 1]) - mean * 1000 * (atm->z[ip] - atm->z[ip - 1]));
  }

  /* Lower part of profile... */
  for (int ip = ipref - 1; ip >= 0; ip--) {
    double mean = 0;
    for (int i = 0; i < ipts; i++) {
      if (ig_h2o >= 0)
        e = LIN(0.0, atm->q[ig_h2o][ip + 1],
```

```
                ipts - 1.0, atm->q[ig_h2o][ip], (double) i);
      mean += (e * mmh2o + (1 - e) * mmair)
        * G0 / RI
        / LIN(0.0, atm->t[ip + 1], ipts - 1.0, atm->t[ip], (double) i) / ipts;
    }

    /* Compute p(z,T)... */
    atm->p[ip] =
      exp(log(atm->p[ip + 1]) - mean * 1000 * (atm->z[ip] - atm->z[ip + 1]));
  }
}

/*****************************************************************************/

void idx2name(
  ctl_t * ctl,
  int idx,
  char *quantity) {

  if (idx == IDXP)
    sprintf(quantity, "PRESSURE");

  if (idx == IDXT)
    sprintf(quantity, "TEMPERATURE");

  for (int ig = 0; ig < ctl->ng; ig++)
    if (idx == IDXQ(ig))
      sprintf(quantity, "%s", ctl->emitter[ig]);

  for (int iw = 0; iw < ctl->nw; iw++)
    if (idx == IDXK(iw))
      sprintf(quantity, "EXTINCT_WINDOW_%d", iw);

  if (idx == IDXCLZ)
    sprintf(quantity, "CLOUD_HEIGHT");

  if (idx == IDXCLDZ)
    sprintf(quantity, "CLOUD_DEPTH");

  for (int icl = 0; icl < ctl->ncl; icl++)
    if (idx == IDXCLK(icl))
      sprintf(quantity, "CLOUD_EXTINCT_%.4f", ctl->clnu[icl]);

  if (idx == IDXSFZ)
    sprintf(quantity, "SURFACE_HEIGHT");

  if (idx == IDXSFP)
    sprintf(quantity, "SURFACE_PRESSURE");

  if (idx == IDXSFT)
    sprintf(quantity, "SURFACE_TEMPERATURE");

  for (int isf = 0; isf < ctl->nsf; isf++)
    if (idx == IDXSFEPS(isf))
      sprintf(quantity, "SURFACE_EMISSIVITY_%.4f", ctl->sfnu[isf]);
}

/*****************************************************************************/

void init_srcfunc(
  ctl_t * ctl,
  tbl_t * tbl) {

  char filename[2 * LEN];

  double f[NSHAPE], nu[NSHAPE];

  int n;

  /* Write info... */
  LOG(1, "Initialize source function table...");

  /* Loop over channels... */
  for (int id = 0; id < ctl->nd; id++) {

    /* Read filter function... */
    sprintf(filename, "%s_%.4f.filt", ctl->tblbase, ctl->nu[id]);
    read_shape(filename, nu, f, &n);

    /* Get minimum grid spacing... */
    double dnu = 1.0;
    for (int i = 1; i < n; i++)
      dnu = GSL_MIN(dnu, nu[i] - nu[i - 1]);

    /* Compute source function table... */
#pragma omp parallel for default(none) shared(ctl,tbl,id,nu,f,n,dnu)
    for (int it = 0; it < TBLNS; it++) {
```

```
      /* Set temperature... */
      tbl->st[it] = LIN(0.0, TMIN, TBLNS - 1.0, TMAX, (double) it);

      /* Integrate Planck function... */
      double fsum = tbl->sr[it][id] = 0;
      for (double fnu = nu[0]; fnu <= nu[n - 1]; fnu += dnu) {
        int i = locate_irr(nu, n, fnu);
        double ff = LIN(nu[i], f[i], nu[i + 1], f[i + 1], fnu);
        fsum += ff;
        tbl->sr[it][id] += ff * planck(tbl->st[it], fnu);
      }
      tbl->sr[it][id] /= fsum;
    }
  }
}

/*****************************************************************************/

void intpol_atm(
  ctl_t * ctl,
  atm_t * atm,
  double z,
  double *p,
  double *t,
  double *q,
  double *k) {

  /* Get array index... */
  int ip = locate_irr(atm->z, atm->np, z);

  /* Interpolate... */
  *p = EXP(atm->z[ip], atm->p[ip], atm->z[ip + 1], atm->p[ip + 1], z);
  *t = LIN(atm->z[ip], atm->t[ip], atm->z[ip + 1], atm->t[ip + 1], z);
  for (int ig = 0; ig < ctl->ng; ig++)
    q[ig] =
      LIN(atm->z[ip], atm->q[ig][ip], atm->z[ip + 1], atm->q[ig][ip + 1], z);
  for (int iw = 0; iw < ctl->nw; iw++)
    k[iw] =
      LIN(atm->z[ip], atm->k[iw][ip], atm->z[ip + 1], atm->k[iw][ip + 1], z);
}

/*****************************************************************************/

void intpol_tbl(
  ctl_t * ctl,
  tbl_t * tbl,
  los_t * los,
  int ip,
  double tau_path[ND][NG],
  double tau_seg[ND]) {

  double eps, u;

  /* Loop over channels... */
  for (int id = 0; id < ctl->nd; id++) {

    /* Initialize... */
    tau_seg[id] = 1;

    /* Loop over emitters.... */
    for (int ig = 0; ig < ctl->ng; ig++) {

      /* Check size of table (pressure)... */
      if (tbl->np[id][ig] < 30)
        eps = 0;

      /* Check transmittance... */
      else if (tau_path[id][ig] < 1e-9)
        eps = 1;

      /* Interpolate... */
      else {

        /* Determine pressure and temperature indices... */
        int ipr = locate_irr(tbl->p[id][ig], tbl->np[id][ig], los->p[ip]);
        int it0 =
          locate_reg(tbl->t[id][ig][ipr], tbl->nt[id][ig][ipr], los->t[ip]);
        int it1 =
          locate_reg(tbl->t[id][ig][ipr + 1], tbl->nt[id][ig][ipr + 1],
                     los->t[ip]);

        /* Check size of table (temperature and column density)... */
        if (tbl->nt[id][ig][ipr] < 2 || tbl->nt[id][ig][ipr + 1] < 2
            || tbl->nu[id][ig][ipr][it0] < 2
            || tbl->nu[id][ig][ipr][it0 + 1] < 2
            || tbl->nu[id][ig][ipr + 1][it1] < 2
```

```
            || tbl->nu[id][ig][ipr + 1][it1 + 1] < 2)
          eps = 0;

        else {

          /* Get emissivities of extended path... */
          u = intpol_tbl_u(tbl, ig, id, ipr, it0, 1 - tau_path[id][ig]);
          double eps00
            = intpol_tbl_eps(tbl, ig, id, ipr, it0, u + los->u[ip][ig]);

          u = intpol_tbl_u(tbl, ig, id, ipr, it0 + 1, 1 - tau_path[id][ig]);
          double eps01 =
            intpol_tbl_eps(tbl, ig, id, ipr, it0 + 1, u + los->u[ip][ig]);

          u = intpol_tbl_u(tbl, ig, id, ipr + 1, it1, 1 - tau_path[id][ig]);
          double eps10 =
            intpol_tbl_eps(tbl, ig, id, ipr + 1, it1, u + los->u[ip][ig]);

          u =
            intpol_tbl_u(tbl, ig, id, ipr + 1, it1 + 1, 1 - tau_path[id][ig]);
          double eps11 =
            intpol_tbl_eps(tbl, ig, id, ipr + 1, it1 + 1, u + los->u[ip][ig]);

          /* Interpolate with respect to temperature... */
          eps00 = LIN(tbl->t[id][ig][ipr][it0], eps00,
                      tbl->t[id][ig][ipr][it0 + 1], eps01, los->t[ip]);
          eps11 = LIN(tbl->t[id][ig][ipr + 1][it1], eps10,
                      tbl->t[id][ig][ipr + 1][it1 + 1], eps11, los->t[ip]);

          /* Interpolate with respect to pressure... */
          eps00 = LIN(tbl->p[id][ig][ipr], eps00,
                      tbl->p[id][ig][ipr + 1], eps11, los->p[ip]);

          /* Check emssivity range... */
          eps00 = GSL_MAX(GSL_MIN(eps00, 1), 0);

          /* Determine segment emissivity... */
          eps = 1 - (1 - eps00) / tau_path[id][ig];
        }
      }

      /* Get transmittance of extended path... */
      tau_path[id][ig] *= (1 - eps);

      /* Get segment transmittance... */
      tau_seg[id] *= (1 - eps);
    }
  }
}

/*****************************************************************************/

double intpol_tbl_eps(
  tbl_t * tbl,
  int ig,
  int id,
  int ip,
  int it,
  double u) {

  /* Lower boundary... */
  if (u < tbl->u[id][ig][ip][it][0])
    return LIN(0, 0, tbl->u[id][ig][ip][it][0], tbl->eps[id][ig][ip][it][0],
               u);

  /* Upper boundary... */
  else if (u > tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1])
    return LIN(tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               1e30, 1, u);

  /* Interpolation... */
  else {

    /* Get index... */
    int idx = locate_tbl(tbl->u[id][ig][ip][it], tbl->nu[id][ig][ip][it], u);

    /* Interpolate... */
    return
      LIN(tbl->u[id][ig][ip][it][idx], tbl->eps[id][ig][ip][it][idx],
          tbl->u[id][ig][ip][it][idx + 1], tbl->eps[id][ig][ip][it][idx + 1],
          u);
  }
}

/*****************************************************************************/
```

```
double intpol_tbl_u(
  tbl_t * tbl,
  int ig,
  int id,
  int ip,
  int it,
  double eps) {

  /* Lower boundary... */
  if (eps < tbl->eps[id][ig][ip][it][0])
    return LIN(0, 0, tbl->eps[id][ig][ip][it][0], tbl->u[id][ig][ip][it][0],
               eps);

  /* Upper boundary... */
  else if (eps > tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1])
    return LIN(tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               1, 1e30, eps);

  /* Interpolation... */
  else {

    /* Get index... */
    int idx
      = locate_tbl(tbl->eps[id][ig][ip][it], tbl->nu[id][ig][ip][it], eps);

    /* Interpolate... */
    return
      LIN(tbl->eps[id][ig][ip][it][idx], tbl->u[id][ig][ip][it][idx],
          tbl->eps[id][ig][ip][it][idx + 1], tbl->u[id][ig][ip][it][idx + 1],
          eps);
  }
}

/*****************************************************************************/

void jsec2time(
  double jsec,
  int *year,
  int *mon,
  int *day,
  int *hour,
  int *min,
  int *sec,
  double *remain) {

  struct tm t0, *t1;

  t0.tm_year = 100;
  t0.tm_mon = 0;
  t0.tm_mday = 1;
  t0.tm_hour = 0;
  t0.tm_min = 0;
  t0.tm_sec = 0;

  time_t jsec0 = (time_t) jsec + timegm(&t0);
  t1 = gmtime(&jsec0);

  *year = t1->tm_year + 1900;
  *mon = t1->tm_mon + 1;
  *day = t1->tm_mday;
  *hour = t1->tm_hour;
  *min = t1->tm_min;
  *sec = t1->tm_sec;
  *remain = jsec - floor(jsec);
}

/*****************************************************************************/

void kernel(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs,
  gsl_matrix * k) {

  atm_t *atm1;
  obs_t *obs1;

  gsl_vector *x0, *x1, *yy0, *yy1;

  int *iqa;

  /* Get sizes... */
  size_t m = k->size1;
  size_t n = k->size2;

  /* Allocate... */
```

```
  x0 = gsl_vector_alloc(n);
  yy0 = gsl_vector_alloc(m);
  ALLOC(iqa, int,
        N);

  /* Compute radiance for undisturbed atmospheric data... */
  formod(ctl, atm, obs);

  /* Compose vectors... */
  atm2x(ctl, atm, x0, iqa, NULL);
  obs2y(ctl, obs, yy0, NULL, NULL);

  /* Initialize kernel matrix... */
  gsl_matrix_set_zero(k);

  /* Loop over state vector elements... */
#pragma omp parallel for default(none) shared(ctl,atm,obs,k,x0,yy0,n,m,iqa) private(x1, yy1, atm1,
 obs1)
  for (size_t j = 0; j < n; j++) {

    /* Allocate... */
    x1 = gsl_vector_alloc(n);
    yy1 = gsl_vector_alloc(m);
    ALLOC(atm1, atm_t, 1);
    ALLOC(obs1, obs_t, 1);

    /* Set perturbation size... */
    double h;
    if (iqa[j] == IDXP)
      h = GSL_MAX(fabs(0.01 * gsl_vector_get(x0, j)), 1e-7);
    else if (iqa[j] == IDXT)
      h = 1.0;
    else if (iqa[j] >= IDXQ(0) && iqa[j] < IDXQ(ctl->ng))
      h = GSL_MAX(fabs(0.01 * gsl_vector_get(x0, j)), 1e-15);
    else if (iqa[j] >= IDXK(0) && iqa[j] < IDXK(ctl->nw))
      h = 1e-4;
    else if (iqa[j] == IDXCLZ || iqa[j] == IDXCLDZ)
      h = 1.0;
    else if (iqa[j] >= IDXCLK(0) && iqa[j] < IDXCLK(ctl->ncl))
      h = 1e-4;
    else if (iqa[j] == IDXSFZ)
      h = 0.1;
    else if (iqa[j] == IDXSFP)
      h = 10.0;
    else if (iqa[j] == IDXSFT)
      h = 1.0;
    else if (iqa[j] >= IDXSFEPS(0) && iqa[j] < IDXSFEPS(ctl->nsf))
      h = 1e-2;
    else
      ERRMSG("Cannot set perturbation size!");

    /* Disturb state vector element... */
    gsl_vector_memcpy(x1, x0);
    gsl_vector_set(x1, j, gsl_vector_get(x1, j) + h);
    copy_atm(ctl, atm1, atm, 0);
    copy_obs(ctl, obs1, obs, 0);
    x2atm(ctl, x1, atm1);

    /* Compute radiance for disturbed atmospheric data... */
    formod(ctl, atm1, obs1);

    /* Compose measurement vector for disturbed radiance data... */
    obs2y(ctl, obs1, yy1, NULL, NULL);

    /* Compute derivatives... */
    for (size_t i = 0; i < m; i++)
      gsl_matrix_set(k, i, j,
                     (gsl_vector_get(yy1, i) - gsl_vector_get(yy0, i)) / h);

    /* Free... */
    gsl_vector_free(x1);
    gsl_vector_free(yy1);
    free(atm1);
    free(obs1);
  }

  /* Free... */
  gsl_vector_free(x0);
  gsl_vector_free(yy0);
  free(iqa);
}

/*****************************************************************************/

int locate_irr(
  double *xx,
  int n,
```

```
  double x) {

  int ilo = 0;
  int ihi = n - 1;
  int i = (ihi + ilo) » 1;

  if (xx[i] < xx[i + 1])
    while (ihi > ilo + 1) {
      i = (ihi + ilo) » 1;
      if (xx[i] > x)
        ihi = i;
      else
        ilo = i;
  } else
    while (ihi > ilo + 1) {
      i = (ihi + ilo) » 1;
      if (xx[i] <= x)
        ihi = i;
      else
        ilo = i;
    }

  return ilo;
}

/*****************************************************************************/

int locate_reg(
  double *xx,
  int n,
  double x) {

  /* Calculate index... */
  int i = (int) ((x - xx[0]) / (xx[1] - xx[0]));

  /* Check range... */
  if (i < 0)
    return 0;
  else if (i > n - 2)
    return n - 2;
  else
    return i;
}

/*****************************************************************************/

int locate_tbl(
  float *xx,
  int n,
  double x) {

  int ilo = 0;
  int ihi = n - 1;
  int i = (ihi + ilo) » 1;

  while (ihi > ilo + 1) {
    i = (ihi + ilo) » 1;
    if (xx[i] > x)
      ihi = i;
    else
      ilo = i;
  }

  return ilo;
}

/*****************************************************************************/

size_t obs2y(
  ctl_t * ctl,
  obs_t * obs,
  gsl_vector * y,
  int *ida,
  int *ira) {

  size_t m = 0;

  /* Determine measurement vector... */
  for (int ir = 0; ir < obs->nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      if (gsl_finite(obs->rad[id][ir])) {
        if (y != NULL)
          gsl_vector_set(y, m, obs->rad[id][ir]);
        if (ida != NULL)
          ida[m] = id;
        if (ira != NULL)
          ira[m] = ir;
```

```
        m++;
      }

  return m;
}

/*****************************************************************************/

double planck(
  double t,
  double nu) {

  return C1 * POW3(nu) / gsl_expm1(C2 * nu / t);
}

/*****************************************************************************/

void raytrace(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs,
  los_t * los,
  int ir) {

  const double h = 0.02, zrefrac = 60;

  double ds, ex0[3], ex1[3], k[NW], lat, lon, n, ng[3], norm,
    p, q[NG], t, x[3], xh[3], xobs[3], xvp[3], z = 1e99, zmax, zmin;

  int stop = 0;

  /* Initialize... */
  los->np = 0;
  los->sft = -999;
  obs->tpz[ir] = obs->vpz[ir];
  obs->tplon[ir] = obs->vplon[ir];
  obs->tplat[ir] = obs->vplat[ir];

  /* Get altitude range of atmospheric data... */
  gsl_stats_minmax(&zmin, &zmax, atm->z, 1, (size_t) atm->np);
  if (ctl->nsf > 0) {
    zmin = GSL_MAX(atm->sfz, zmin);
    if (atm->sfp > 0) {
      int ip = locate_irr(atm->p, atm->np, atm->sfp);
      double zip = LIN(log(atm->p[ip]), atm->z[ip],
                       log(atm->p[ip + 1]), atm->z[ip + 1], log(atm->sfp));
      zmin = GSL_MAX(zip, zmin);
    }
  }

  /* Check observer altitude... */
  if (obs->obsz[ir] < zmin)
    ERRMSG("Observer below surface!");

  /* Check view point altitude... */
  if (obs->vpz[ir] > zmax)
    return;

  /* Determine Cartesian coordinates for observer and view point... */
  geo2cart(obs->obsz[ir], obs->obslon[ir], obs->obslat[ir], xobs);
  geo2cart(obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], xvp);

  /* Determine initial tangent vector... */
  for (int i = 0; i < 3; i++)
    ex0[i] = xvp[i] - xobs[i];
  norm = NORM(ex0);
  for (int i = 0; i < 3; i++)
    ex0[i] /= norm;

  /* Observer within atmosphere... */
  for (int i = 0; i < 3; i++)
    x[i] = xobs[i];

  /* Observer above atmosphere (search entry point)... */
  if (obs->obsz[ir] > zmax) {
    double dmax = norm, dmin = 0;
    while (fabs(dmin - dmax) > 0.001) {
      double d = (dmax + dmin) / 2;
      for (int i = 0; i < 3; i++)
        x[i] = xobs[i] + d * ex0[i];
      cart2geo(x, &z, &lon, &lat);
      if (z <= zmax && z > zmax - 0.001)
        break;
      if (z < zmax - 0.0005)
        dmax = d;
      else
        dmin = d;
```

```
    }
  }

  /* Ray-tracing... */
  while (1) {

    /* Set step length... */
    ds = ctl->rayds;
    if (ctl->raydz > 0) {
      norm = NORM(x);
      for (int i = 0; i < 3; i++)
        xh[i] = x[i] / norm;
      double cosa = fabs(DOTP(ex0, xh));
      if (cosa != 0)
        ds = GSL_MIN(ctl->rayds, ctl->raydz / cosa);
    }

    /* Determine geolocation... */
    cart2geo(x, &z, &lon, &lat);

    /* Check if LOS hits the ground or has left atmosphere... */
    if (z < zmin || z > zmax) {
      stop = (z < zmin ? 2 : 1);
      double frac =
        ((z <
          zmin ? zmin : zmax) - los->z[los->np - 1]) / (z - los->z[los->np -
                                                                    1]);
      geo2cart(los->z[los->np - 1], los->lon[los->np - 1],
               los->lat[los->np - 1], xh);
      for (int i = 0; i < 3; i++)
        x[i] = xh[i] + frac * (x[i] - xh[i]);
      cart2geo(x, &z, &lon, &lat);
      los->ds[los->np - 1] = ds * frac;
      ds = 0;
    }

    /* Interpolate atmospheric data... */
    intpol_atm(ctl, atm, z, &p, &t, q, k);

    /* Save data... */
    los->lon[los->np] = lon;
    los->lat[los->np] = lat;
    los->z[los->np] = z;
    los->p[los->np] = p;
    los->t[los->np] = t;
    for (int ig = 0; ig < ctl->ng; ig++)
      los->q[los->np][ig] = q[ig];
    for (int id = 0; id < ctl->nd; id++)
      los->k[los->np][id] = k[ctl->window[id]];
    los->ds[los->np] = ds;

    /* Add cloud extinction... */
    if (ctl->ncl > 0 && atm->cldz > 0) {
      double aux = exp(-0.5 * POW2((z - atm->clz) / atm->cldz));
      for (int id = 0; id < ctl->nd; id++) {
        int icl = locate_irr(ctl->clnu, ctl->ncl, ctl->nu[id]);
        los->k[los->np][id]
          += aux * LIN(ctl->clnu[icl], atm->clk[icl],
                       ctl->clnu[icl + 1], atm->clk[icl + 1], ctl->nu[id]);
      }
    }

    /* Increment and check number of LOS points... */
    if ((++los->np) > NLOS)
      ERRMSG("Too many LOS points!");

    /* Check stop flag... */
    if (stop) {

      /* Set surface temperature... */
      if (ctl->nsf > 0 && atm->sft > 0)
        t = atm->sft;
      los->sft = (stop == 2 ? t : -999);

      /* Set surface emissivity... */
      for (int id = 0; id < ctl->nd; id++) {
        los->sfeps[id] = 1.0;
        if (ctl->nsf > 0) {
          int isf = locate_irr(ctl->sfnu, ctl->nsf, ctl->nu[id]);
          los->sfeps[id] = LIN(ctl->sfnu[isf], atm->sfeps[isf],
                               ctl->sfnu[isf + 1], atm->sfeps[isf + 1],
                               ctl->nu[id]);
        }
      }

      /* Leave raytracer... */
      break;
```

```
    }

    /* Determine refractivity... */
    if (ctl->refrac && z <= zrefrac)
      n = 1 + refractivity(p, t);
    else
      n = 1;

    /* Construct new tangent vector (first term)... */
    for (int i = 0; i < 3; i++)
      ex1[i] = ex0[i] * n;

    /* Compute gradient of refractivity... */
    if (ctl->refrac && z <= zrefrac) {
      for (int i = 0; i < 3; i++)
        xh[i] = x[i] + 0.5 * ds * ex0[i];
      cart2geo(xh, &z, &lon, &lat);
      intpol_atm(ctl, atm, z, &p, &t, q, k);
      n = refractivity(p, t);
      for (int i = 0; i < 3; i++) {
        xh[i] += h;
        cart2geo(xh, &z, &lon, &lat);
        intpol_atm(ctl, atm, z, &p, &t, q, k);
        ng[i] = (refractivity(p, t) - n) / h;
        xh[i] -= h;
      }
    } else
      for (int i = 0; i < 3; i++)
        ng[i] = 0;

    /* Construct new tangent vector (second term)... */
    for (int i = 0; i < 3; i++)
      ex1[i] += ds * ng[i];

    /* Normalize new tangent vector... */
    norm = NORM(ex1);
    for (int i = 0; i < 3; i++)
      ex1[i] /= norm;

    /* Determine next point of LOS... */
    for (int i = 0; i < 3; i++)
      x[i] += 0.5 * ds * (ex0[i] + ex1[i]);

    /* Copy tangent vector... */
    for (int i = 0; i < 3; i++)
      ex0[i] = ex1[i];
  }

  /* Get tangent point (to be done before changing segment lengths!)... */
  tangent_point(los, &obs->tpz[ir], &obs->tplon[ir], &obs->tplat[ir]);

  /* Change segment lengths according to trapezoid rule... */
  for (int ip = los->np - 1; ip >= 1; ip--)
    los->ds[ip] = 0.5 * (los->ds[ip - 1] + los->ds[ip]);
  los->ds[0] *= 0.5;

  /* Compute column density... */
  for (int ip = 0; ip < los->np; ip++)
    for (int ig = 0; ig < ctl->ng; ig++)
      los->u[ip][ig] = 10 * los->q[ip][ig] * los->p[ip]
        / (KB * los->t[ip]) * los->ds[ip];
}

/*****************************************************************************/

void read_atm(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  atm_t * atm) {

  FILE *in;

  char file[LEN], line[LEN], *tok;

  /* Init... */
  atm->np = 0;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read atmospheric data: %s", file);

```

```
  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read line... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    TOK(line, tok, "%lg", atm->time[atm->np]);
    TOK(NULL, tok, "%lg", atm->z[atm->np]);
    TOK(NULL, tok, "%lg", atm->lon[atm->np]);
    TOK(NULL, tok, "%lg", atm->lat[atm->np]);
    TOK(NULL, tok, "%lg", atm->p[atm->np]);
    TOK(NULL, tok, "%lg", atm->t[atm->np]);
    for (int ig = 0; ig < ctl->ng; ig++)
      TOK(NULL, tok, "%lg", atm->q[ig][atm->np]);
    for (int iw = 0; iw < ctl->nw; iw++)
      TOK(NULL, tok, "%lg", atm->k[iw][atm->np]);
    if (ctl->ncl > 0 && atm->np == 0) {
      TOK(NULL, tok, "%lg", atm->clz);
      TOK(NULL, tok, "%lg", atm->cldz);
      for (int icl = 0; icl < ctl->ncl; icl++)
        TOK(NULL, tok, "%lg", atm->clk[icl]);
    }
    if (ctl->nsf > 0 && atm->np == 0) {
      TOK(NULL, tok, "%lg", atm->sfz);
      TOK(NULL, tok, "%lg", atm->sfp);
      TOK(NULL, tok, "%lg", atm->sft);
      for (int isf = 0; isf < ctl->nsf; isf++)
        TOK(NULL, tok, "%lg", atm->sfeps[isf]);
    }

    /* Increment data point counter... */
    if ((++atm->np) > NP)
      ERRMSG("Too many data points!");
  }

  /* Close file... */
  fclose(in);

  /* Check number of points... */
  if (atm->np < 1)
    ERRMSG("Could not read any data!");
}

/*****************************************************************************/

void read_ctl(
  int argc,
  char *argv[],
  ctl_t * ctl) {

  /* Write info... */
  LOG(1, "\nJuelich Rapid Spectral Simulation Code (JURASSIC)\n"
      "(executable: %s | version: %s | compiled: %s, %s)\n",
      argv[0], VERSION, __DATE__, __TIME__);

  /* Emitters... */
  ctl->ng = (int) scan_ctl(argc, argv, "NG", -1, "0", NULL);
  if (ctl->ng < 0 || ctl->ng > NG)
    ERRMSG("Set 0 <= NG <= MAX!");
  for (int ig = 0; ig < ctl->ng; ig++)
    scan_ctl(argc, argv, "EMITTER", ig, "", ctl->emitter[ig]);

  /* Radiance channels... */
  ctl->nd = (int) scan_ctl(argc, argv, "ND", -1, "0", NULL);
  if (ctl->nd < 0 || ctl->nd > ND)
    ERRMSG("Set 0 <= ND <= MAX!");
  for (int id = 0; id < ctl->nd; id++)
    ctl->nu[id] = scan_ctl(argc, argv, "NU", id, "", NULL);

  /* Spectral windows... */
  ctl->nw = (int) scan_ctl(argc, argv, "NW", -1, "1", NULL);
  if (ctl->nw < 0 || ctl->nw > NW)
    ERRMSG("Set 0 <= NW <= MAX!");
  for (int id = 0; id < ctl->nd; id++)
    ctl->window[id] = (int) scan_ctl(argc, argv, "WINDOW", id, "0", NULL);

  /* Cloud data... */
  ctl->ncl = (int) scan_ctl(argc, argv, "NCL", -1, "0", NULL);
  if (ctl->ncl < 0 || ctl->ncl > NCL)
    ERRMSG("Set 0 <= NCL <= MAX!");
  if (ctl->ncl == 1)
    ERRMSG("Set NCL > 1!");
  for (int icl = 0; icl < ctl->ncl; icl++)
    ctl->clnu[icl] = scan_ctl(argc, argv, "CLNU", icl, "", NULL);

```

```
  /* Surface data... */
  ctl->nsf = (int) scan_ctl(argc, argv, "NSF", -1, "0", NULL);
  if (ctl->nsf < 0 || ctl->nsf > NSF)
    ERRMSG("Set 0 <= NSF <= MAX!");
  if (ctl->nsf == 1)
    ERRMSG("Set NSF > 1!");
  for (int isf = 0; isf < ctl->nsf; isf++)
    ctl->sfnu[isf] = scan_ctl(argc, argv, "SFNU", isf, "", NULL);
  ctl->sftype = (int) scan_ctl(argc, argv, "SFTYPE", -1, "2", NULL);
  if (ctl->sftype < 0 || ctl->sftype > 3)
    ERRMSG("Set 0 <= SFTYPE <= 3!");
  ctl->sfsza = scan_ctl(argc, argv, "SFSZA", -1, "-999", NULL);

  /* Emissivity look-up tables... */
  scan_ctl(argc, argv, "TBLBASE", -1, "-", ctl->tblbase);
  ctl->tblfmt = (int) scan_ctl(argc, argv, "TBLFMT", -1, "1", NULL);

  /* Hydrostatic equilibrium... */
  ctl->hydz = scan_ctl(argc, argv, "HYDZ", -1, "-999", NULL);

  /* Continua... */
  ctl->ctm_co2 = (int) scan_ctl(argc, argv, "CTM_CO2", -1, "1", NULL);
  ctl->ctm_h2o = (int) scan_ctl(argc, argv, "CTM_H2O", -1, "1", NULL);
  ctl->ctm_n2 = (int) scan_ctl(argc, argv, "CTM_N2", -1, "1", NULL);
  ctl->ctm_o2 = (int) scan_ctl(argc, argv, "CTM_O2", -1, "1", NULL);

  /* Ray-tracing... */
  ctl->refrac = (int) scan_ctl(argc, argv, "REFRAC", -1, "1", NULL);
  ctl->rayds = scan_ctl(argc, argv, "RAYDS", -1, "10", NULL);
  ctl->raydz = scan_ctl(argc, argv, "RAYDZ", -1, "0.1", NULL);

  /* Field of view... */
  scan_ctl(argc, argv, "FOV", -1, "-", ctl->fov);

  /* Retrieval interface... */
  ctl->retp_zmin = scan_ctl(argc, argv, "RETP_ZMIN", -1, "-999", NULL);
  ctl->retp_zmax = scan_ctl(argc, argv, "RETP_ZMAX", -1, "-999", NULL);
  ctl->rett_zmin = scan_ctl(argc, argv, "RETT_ZMIN", -1, "-999", NULL);
  ctl->rett_zmax = scan_ctl(argc, argv, "RETT_ZMAX", -1, "-999", NULL);
  for (int ig = 0; ig < ctl->ng; ig++) {
    ctl->retq_zmin[ig] = scan_ctl(argc, argv, "RETQ_ZMIN", ig, "-999", NULL);
    ctl->retq_zmax[ig] = scan_ctl(argc, argv, "RETQ_ZMAX", ig, "-999", NULL);
  }
  for (int iw = 0; iw < ctl->nw; iw++) {
    ctl->retk_zmin[iw] = scan_ctl(argc, argv, "RETK_ZMIN", iw, "-999", NULL);
    ctl->retk_zmax[iw] = scan_ctl(argc, argv, "RETK_ZMAX", iw, "-999", NULL);
  }
  ctl->ret_clz = (int) scan_ctl(argc, argv, "RET_CLZ", -1, "0", NULL);
  ctl->ret_cldz = (int) scan_ctl(argc, argv, "RET_CLDZ", -1, "0", NULL);
  ctl->ret_clk = (int) scan_ctl(argc, argv, "RET_CLK", -1, "0", NULL);
  ctl->ret_sfz = (int) scan_ctl(argc, argv, "RET_SFZ", -1, "0", NULL);
  ctl->ret_sfp = (int) scan_ctl(argc, argv, "RET_SFP", -1, "0", NULL);
  ctl->ret_sft = (int) scan_ctl(argc, argv, "RET_SFT", -1, "0", NULL);
  ctl->ret_sfeps = (int) scan_ctl(argc, argv, "RET_SFEPS", -1, "0", NULL);

  /* Output flags... */
  ctl->write_bbt = (int) scan_ctl(argc, argv, "WRITE_BBT", -1, "0", NULL);
  ctl->write_matrix =
    (int) scan_ctl(argc, argv, "WRITE_MATRIX", -1, "0", NULL);

  /* External forward models... */
  ctl->formod = (int) scan_ctl(argc, argv, "FORMOD", -1, "1", NULL);
  scan_ctl(argc, argv, "RFMBIN", -1, "-", ctl->rfmbin);
  scan_ctl(argc, argv, "RFMHIT", -1, "-", ctl->rfmhit);
  for (int ig = 0; ig < ctl->ng; ig++)
    scan_ctl(argc, argv, "RFMXSC", ig, "-", ctl->rfmxsc[ig]);
}

/*****************************************************************************/

void read_matrix(
  const char *dirname,
  const char *filename,
  gsl_matrix * matrix) {

  FILE *in;

  char dum[LEN], file[LEN], line[LEN];

  double value;

  int i, j;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
```

```
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read matrix: %s", file);

  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read data... */
  gsl_matrix_set_zero(matrix);
  while (fgets(line, LEN, in))
    if (sscanf(line, "%d %s %s %s %s %s %d %s %s %s %s %s %lg",
               &i, dum, dum, dum, dum, dum,
               &j, dum, dum, dum, dum, dum, &value) == 13)
      gsl_matrix_set(matrix, (size_t) i, (size_t) j, value);

  /* Close file... */
  fclose(in);
}

/*****************************************************************************/

void read_obs(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  obs_t * obs) {

  FILE *in;

  char file[LEN], line[LEN], *tok;

  /* Init... */
  obs->nr = 0;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read observation data: %s", file);

  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read line... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    TOK(line, tok, "%lg", obs->time[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obsz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obslon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obslat[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vpz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vplon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vplat[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tpz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tplon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tplat[obs->nr]);
    for (int id = 0; id < ctl->nd; id++)
      TOK(NULL, tok, "%lg", obs->rad[id][obs->nr]);
    for (int id = 0; id < ctl->nd; id++)
      TOK(NULL, tok, "%lg", obs->tau[id][obs->nr]);

    /* Increment counter... */
    if ((++obs->nr) > NR)
      ERRMSG("Too many rays!");
  }

  /* Close file... */
  fclose(in);

  /* Check number of points... */
  if (obs->nr < 1)
    ERRMSG("Could not read any data!");
}

/*****************************************************************************/

double read_obs_rfm(
  const char *basename,
  double z,
  double *nu,
```

```
  double *f,
  int n) {

  FILE *in;

  char filename[LEN];

  double filt, fsum = 0, nu2[NSHAPE], *nurfm, *rad, radsum = 0;

  int i, idx, ipts, npts;

  /* Allocate... */
  ALLOC(nurfm, double,
        RFMNPTS);
  ALLOC(rad, double,
        RFMNPTS);

  /* Search RFM spectrum... */
  sprintf(filename, "%s_%05d.asc", basename, (int) (z * 1000));
  if (!(in = fopen(filename, "r"))) {
    sprintf(filename, "%s_%05d.asc", basename, (int) (z * 1000) + 1);
    if (!(in = fopen(filename, "r")))
      ERRMSG("Cannot find RFM data file!");
  }
  fclose(in);

  /* Read RFM spectrum... */
  read_rfm_spec(filename, nurfm, rad, &npts);

  /* Set wavenumbers... */
  nu2[0] = nu[0];
  nu2[n - 1] = nu[n - 1];
  for (i = 1; i < n - 1; i++)
    nu2[i] = LIN(0.0, nu2[0], n - 1.0, nu2[n - 1], i);

  /* Convolute... */
  for (ipts = 0; ipts < npts; ipts++)
    if (nurfm[ipts] >= nu2[0] && nurfm[ipts] <= nu2[n - 1]) {
      idx = locate_irr(nu2, n, nurfm[ipts]);
      filt = LIN(nu2[idx], f[idx], nu2[idx + 1], f[idx + 1], nurfm[ipts]);
      fsum += filt;
      radsum += filt * rad[ipts];
    }

  /* Free... */
  free(nurfm);
  free(rad);

  /* Return radiance... */
  return radsum / fsum;
}

/*****************************************************************************/

void read_rfm_spec(
  const char *filename,
  double *nu,
  double *rad,
  int *npts) {

  FILE *in;

  char line[RFMLINE], *tok;

  double dnu, nu0, nu1;

  int i, ipts = 0;

  /* Write info... */
  printf("Read RFM data: %s\n", filename);

  /* Open file... */
  if (!(in = fopen(filename, "r")))
    ERRMSG("Cannot open file!");

  /* Read header...... */
  for (i = 0; i < 4; i++)
    if (fgets(line, RFMLINE, in) == NULL)
      ERRMSG("Error while reading file header!");
  sscanf(line, "%d %lg %lg %lg", npts, &nu0, &dnu, &nu1);
  if (*npts > RFMNPTS)
    ERRMSG("Too many spectral grid points!");

  /* Read radiance data... */
  while (fgets(line, RFMLINE, in) && ipts < *npts - 1) {
    if ((tok = strtok(line, " \t\n")) != NULL)
      if (sscanf(tok, "%lg", &rad[ipts]) == 1)
```

```
        ipts++;
    while ((tok = strtok(NULL, " \t\n")) != NULL)
      if (sscanf(tok, "%lg", &rad[ipts]) == 1)
        ipts++;
  }
  if (ipts != *npts)
    ERRMSG("Error while reading RFM data!");

  /* Compute wavenumbers... */
  for (ipts = 0; ipts < *npts; ipts++)
    nu[ipts] = LIN(0.0, nu0, (double) (*npts - 1), nu1, (double) ipts);

  /* Close file... */
  fclose(in);
}

/*****************************************************************************/

void read_shape(
  const char *filename,
  double *x,
  double *y,
  int *n) {

  FILE *in;

  char line[LEN];

  /* Write info... */
  LOG(1, "Read shape function: %s", filename);

  /* Open file... */
  if (!(in = fopen(filename, "r")))
    ERRMSG("Cannot open file!");

  /* Read data... */
  *n = 0;
  while (fgets(line, LEN, in))
    if (sscanf(line, "%lg %lg", &x[*n], &y[*n]) == 2)
      if ((++(*n)) > NSHAPE)
        ERRMSG("Too many data points!");

  /* Check number of points... */
  if (*n < 1)
    ERRMSG("Could not read any data!");

  /* Close file... */
  fclose(in);
}

/*****************************************************************************/

void read_tbl(
  ctl_t * ctl,
  tbl_t * tbl) {

  FILE *in;

  char filename[2 * LEN], line[LEN];

  double eps, press, temp, u;

  /* Loop over trace gases and channels... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ig = 0; ig < ctl->ng; ig++) {

      /* Initialize... */
      tbl->np[id][ig] = -1;
      double eps_old = -999;
      double press_old = -999;
      double temp_old = -999;
      double u_old = -999;

      /* Set filename... */
      sprintf(filename, "%s_%.4f_%s.%s", ctl->tblbase,
              ctl->nu[id], ctl->emitter[ig],
              ctl->tblfmt == 1 ? "tab" : "bin");

      /* Write info... */
      LOG(1, "Read emissivity table: %s", filename);

      /* Try to open file... */
      if (!(in = fopen(filename, "r"))) {
        WARN("Missing emissivity table: %s", filename);
        continue;
      }

```

```
  /* Read ASCII tables... */
  if (ctl->tblfmt == 1) {

    /* Read data... */
    while (fgets(line, LEN, in)) {

      /* Parse line... */
      if (sscanf(line, "%lg %lg %lg %lg", &press, &temp, &u, &eps) != 4)
        continue;

      /* Check ranges... */
      if (u < 0 || u > 1e30 || eps < 0 || eps > 1)
        continue;

      /* Determine pressure index... */
      if (press != press_old) {
        press_old = press;
        if ((++tbl->np[id][ig]) >= TBLNP)
          ERRMSG("Too many pressure levels!");
        tbl->nt[id][ig][tbl->np[id][ig]] = -1;
      }

      /* Determine temperature index... */
      if (temp != temp_old) {
        temp_old = temp;
        if ((++tbl->nt[id][ig][tbl->np[id][ig]]) >= TBLNT)
          ERRMSG("Too many temperatures!");
        tbl->nu[id][ig][tbl->np[id][ig]]
          [tbl->nt[id][ig][tbl->np[id][ig]]] = -1;
      }

      /* Determine column density index... */
      if ((eps > eps_old && u > u_old) || tbl->nu[id][ig][tbl->np[id][ig]]
          [tbl->nt[id][ig][tbl->np[id][ig]]] < 0) {
        eps_old = eps;
        u_old = u;
        if ((++tbl->nu[id][ig][tbl->np[id][ig]]
             [tbl->nt[id][ig][tbl->np[id][ig]]]) >= TBLNU) {
          tbl->nu[id][ig][tbl->np[id][ig]]
            [tbl->nt[id][ig][tbl->np[id][ig]]]--;
          continue;
        }
      }

      /* Store data... */
      tbl->p[id][ig][tbl->np[id][ig]] = press;
      tbl->t[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
        = temp;
      tbl->u[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
        [tbl->nu[id][ig][tbl->np[id][ig]]
         [tbl->nt[id][ig][tbl->np[id][ig]]]] = (float) u;
      tbl->eps[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
        [tbl->nu[id][ig][tbl->np[id][ig]]
         [tbl->nt[id][ig][tbl->np[id][ig]]]] = (float) eps;
    }

    /* Increment counters... */
    tbl->np[id][ig]++;
    for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
      tbl->nt[id][ig][ip]++;
      for (int it = 0; it < tbl->nt[id][ig][ip]; it++)
        tbl->nu[id][ig][ip][it]++;
    }
  }

  /* Read binary data... */
  else if (ctl->tblfmt == 2) {

    /* Read data... */
    FREAD(&tbl->np[id][ig], int,
          1,
          in);
    if (tbl->np[id][ig] > TBLNP)
      ERRMSG("Too many pressure levels!");
    FREAD(tbl->p[id][ig], double,
            (size_t) tbl->np[id][ig],
          in);
    for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
      FREAD(&tbl->nt[id][ig][ip], int,
            1,
            in);
      if (tbl->nt[id][ig][ip] > TBLNT)
        ERRMSG("Too many temperatures!");
      FREAD(tbl->t[id][ig][ip], double,
              (size_t) tbl->nt[id][ig][ip],
            in);
      for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
```

```
            FREAD(&tbl->nu[id][ig][ip][it], int,
                  1,
                  in);
            if (tbl->nu[id][ig][ip][it] > TBLNU)
              ERRMSG("Too many column densities!");
            FREAD(tbl->u[id][ig][ip][it], float,
                    (size_t) tbl->nu[id][ig][ip][it],
                  in);
            FREAD(tbl->eps[id][ig][ip][it], float,
                    (size_t) tbl->nu[id][ig][ip][it],
                  in);
          }
        }
      }

      /* Error message... */
      else
        ERRMSG("Unknown look-up table format!");

      /* Close file... */
      fclose(in);
    }
}

/*****************************************************************************/

double refractivity(
  double p,
  double t) {

  /* Refractivity of air at 4 to 15 micron... */
  return 7.753e-05 * p / t;
}

/*****************************************************************************/

double scan_ctl(
  int argc,
  char *argv[],
  const char *varname,
  int arridx,
  const char *defvalue,
  char *value) {

  FILE *in = NULL;

  char dummy[LEN], fullname1[LEN], fullname2[LEN], line[LEN],
    rvarname[LEN], rval[LEN];

  int contain = 0;

  /* Open file... */
  if (argv[1][0] != '-')
    if (!(in = fopen(argv[1], "r")))
      ERRMSG("Cannot open file!");

  /* Set full variable name... */
  if (arridx >= 0) {
    sprintf(fullname1, "%s[%d]", varname, arridx);
    sprintf(fullname2, "%s[*]", varname);
  } else {
    sprintf(fullname1, "%s", varname);
    sprintf(fullname2, "%s", varname);
  }

  /* Read data... */
  if (in != NULL)
    while (fgets(line, LEN, in))
      if (sscanf(line, "%s %s %s", rvarname, dummy, rval) == 3)
        if (strcasecmp(rvarname, fullname1) == 0 ||
            strcasecmp(rvarname, fullname2) == 0) {
          contain = 1;
          break;
        }
  for (int i = 1; i < argc - 1; i++)
    if (strcasecmp(argv[i], fullname1) == 0 ||
        strcasecmp(argv[i], fullname2) == 0) {
      sprintf(rval, "%s", argv[i + 1]);
      contain = 1;
      break;
    }

  /* Close file... */
  if (in != NULL)
    fclose(in);

  /* Check for missing variables... */
```

```
  if (!contain) {
    if (strlen(defvalue) > 0)
      sprintf(rval, "%s", defvalue);
    else
      ERRMSG("Missing variable %s!\n", fullname1);
  }

  /* Write info... */
  LOG(1, "%s = %s", fullname1, rval);

  /* Return values... */
  if (value != NULL)
    sprintf(value, "%s", rval);
  return atof(rval);
}

/*****************************************************************************/

double sza(
  double sec,
  double lon,
  double lat) {

  /* Number of days and fraction with respect to 2000-01-01T12:00Z... */
  double D = sec / 86400 - 0.5;

  /* Geocentric apparent ecliptic longitude [rad]... */
  double g = (357.529 + 0.98560028 * D) * M_PI / 180;
  double q = 280.459 + 0.98564736 * D;
  double L = (q + 1.915 * sin(g) + 0.020 * sin(2 * g)) * M_PI / 180;

  /* Mean obliquity of the ecliptic [rad]... */
  double e = (23.439 - 0.00000036 * D) * M_PI / 180;

  /* Declination [rad]... */
  double dec = asin(sin(e) * sin(L));

  /* Right ascension [rad]... */
  double ra = atan2(cos(e) * sin(L), cos(L));

  /* Greenwich Mean Sidereal Time [h]... */
  double GMST = 18.697374558 + 24.06570982441908 * D;

  /* Local Sidereal Time [h]... */
  double LST = GMST + lon / 15;

  /* Hour angle [rad]... */
  double h = LST / 12 * M_PI - ra;

  /* Convert latitude... */
  lat *= M_PI / 180;

  /* Return solar zenith angle [deg]... */
  return acos(sin(lat) * sin(dec) +
              cos(lat) * cos(dec) * cos(h)) * 180 / M_PI;
}

/*****************************************************************************/

void tangent_point(
  los_t * los,
  double *tpz,
  double *tplon,
  double *tplat) {

  double dummy, v[3], v0[3], v2[3];

  /* Find minimum altitude... */
  size_t ip = gsl_stats_min_index(los->z, 1, (size_t) los->np);

  /* Nadir or zenith... */
  if (ip <= 0 || ip >= (size_t) los->np - 1) {
    *tpz = los->z[los->np - 1];
    *tplon = los->lon[los->np - 1];
    *tplat = los->lat[los->np - 1];
  }

  /* Limb... */
  else {

    /* Determine interpolating polynomial y=a*x^2+b*x+c... */
    double yy0 = los->z[ip - 1];
    double yy1 = los->z[ip];
    double yy2 = los->z[ip + 1];
    double x1 = sqrt(POW2(los->ds[ip]) - POW2(yy1 - yy0));
    double x2 = x1 + sqrt(POW2(los->ds[ip + 1]) - POW2(yy2 - yy1));
    double a = 1 / (x1 - x2) * (-(yy0 - yy1) / x1 + (yy0 - yy2) / x2);
```

```
    double b = -(yy0 - yy1) / x1 - a * x1;
    double c = yy0;

    /* Get tangent point location... */
    double x = -b / (2 * a);
    *tpz = a * x * x + b * x + c;
    geo2cart(los->z[ip - 1], los->lon[ip - 1], los->lat[ip - 1], v0);
    geo2cart(los->z[ip + 1], los->lon[ip + 1], los->lat[ip + 1], v2);
    for (int i = 0; i < 3; i++)
      v[i] = LIN(0.0, v0[i], x2, v2[i], x);
    cart2geo(v, &dummy, tplon, tplat);
  }
}

/*****************************************************************************/

void time2jsec(
  int year,
  int mon,
  int day,
  int hour,
  int min,
  int sec,
  double remain,
  double *jsec) {

  struct tm t0, t1;

  t0.tm_year = 100;
  t0.tm_mon = 0;
  t0.tm_mday = 1;
  t0.tm_hour = 0;
  t0.tm_min = 0;
  t0.tm_sec = 0;

  t1.tm_year = year - 1900;
  t1.tm_mon = mon - 1;
  t1.tm_mday = day;
  t1.tm_hour = hour;
  t1.tm_min = min;
  t1.tm_sec = sec;

  *jsec = (double) timegm(&t1) - (double) timegm(&t0) + remain;
}

/*****************************************************************************/

void timer(
  const char *name,
  const char *file,
  const char *func,
  int line,
  int mode) {

  static double w0[10];

  static int l0[10], nt;

  /* Start new timer... */
  if (mode == 1) {
    w0[nt] = omp_get_wtime();
    l0[nt] = line;
    if ((++nt) >= 10)
      ERRMSG("Too many timers!");
  }

  /* Write elapsed time... */
  else {

    /* Check timer index... */
    if (nt - 1 < 0)
      ERRMSG("Coding error!");

    /* Write elapsed time... */
    LOG(1, "Timer '%s' (%s, %s, l%d-%d): %.3f sec",
        name, file, func, l0[nt - 1], line, omp_get_wtime() - w0[nt - 1]);
  }

  /* Stop timer... */
  if (mode == 3)
    nt--;
}

/*****************************************************************************/

void write_atm(
  const char *dirname,
```

```
  const char *filename,
  ctl_t * ctl,
  atm_t * atm) {

  FILE *out;

  char file[LEN];

  int n = 6;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write atmospheric data: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = altitude [km]\n"
          "# $3 = longitude [deg]\n"
          "# $4 = latitude [deg]\n"
          "# $5 = pressure [hPa]\n" "# $6 = temperature [K]\n");
  for (int ig = 0; ig < ctl->ng; ig++)
    fprintf(out, "# $%d = %s volume mixing ratio [ppv]\n",
            ++n, ctl->emitter[ig]);
  for (int iw = 0; iw < ctl->nw; iw++)
    fprintf(out, "# $%d = extinction (window %d) [1/km]\n", ++n, iw);
  if (ctl->ncl > 0) {
    fprintf(out, "# $%d = cloud layer height [km]\n", ++n);
    fprintf(out, "# $%d = cloud layer depth [km]\n", ++n);
    for (int icl = 0; icl < ctl->ncl; icl++)
      fprintf(out, "# $%d = cloud layer extinction (%.4f cm^-1) [1/km]\n",
              ++n, ctl->clnu[icl]);
  }
  if (ctl->nsf > 0) {
    fprintf(out, "# $%d = surface layer height [km]\n", ++n);
    fprintf(out, "# $%d = surface layer pressure [hPa]\n", ++n);
    fprintf(out, "# $%d = surface layer temperature [K]\n", ++n);
    for (int isf = 0; isf < ctl->nsf; isf++)
      fprintf(out, "# $%d = surface layer emissivity (%.4f cm^-1)\n",
              ++n, ctl->sfnu[isf]);
  }

  /* Write data... */
  for (int ip = 0; ip < atm->np; ip++) {
    if (ip == 0 || atm->time[ip] != atm->time[ip - 1])
      fprintf(out, "\n");
    fprintf(out, "%.2f %g %g %g %g %g", atm->time[ip], atm->z[ip],
            atm->lon[ip], atm->lat[ip], atm->p[ip], atm->t[ip]);
    for (int ig = 0; ig < ctl->ng; ig++)
      fprintf(out, " %g", atm->q[ig][ip]);
    for (int iw = 0; iw < ctl->nw; iw++)
      fprintf(out, " %g", atm->k[iw][ip]);
    if (ctl->ncl > 0) {
      fprintf(out, " %g %g", atm->clz, atm->cldz);
      for (int icl = 0; icl < ctl->ncl; icl++)
        fprintf(out, " %g", atm->clk[icl]);
    }
    if (ctl->nsf > 0) {
      fprintf(out, " %g %g %g", atm->sfz, atm->sfp, atm->sft);
      for (int isf = 0; isf < ctl->nsf; isf++)
        fprintf(out, " %g", atm->sfeps[isf]);
    }
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);
}

/*****************************************************************************/

void write_atm_rfm(
  const char *filename,
  ctl_t * ctl,
  atm_t * atm) {

  FILE *out;

```

```
  int ig, ip;

  /* Write info... */
  printf("Write RFM data: %s\n", filename);

  /* Create file... */
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create file!");

  /* Write data... */
  fprintf(out, "%d\n", atm->np);
  fprintf(out, "*HGT [km]\n");
  for (ip = 0; ip < atm->np; ip++)
    fprintf(out, "%g\n", atm->z[ip]);
  fprintf(out, "*PRE [mb]\n");
  for (ip = 0; ip < atm->np; ip++)
    fprintf(out, "%g\n", atm->p[ip]);
  fprintf(out, "*TEM [K]\n");
  for (ip = 0; ip < atm->np; ip++)
    fprintf(out, "%g\n", atm->t[ip]);
  for (ig = 0; ig < ctl->ng; ig++) {
    fprintf(out, "*%s [ppmv]\n", ctl->emitter[ig]);
    for (ip = 0; ip < atm->np; ip++)
      fprintf(out, "%g\n", atm->q[ig][ip] * 1e6);
  }
  fprintf(out, "*END\n");

  /* Close file... */
  fclose(out);
}

/*****************************************************************************/

void write_matrix(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  gsl_matrix * matrix,
  atm_t * atm,
  obs_t * obs,
  const char *rowspace,
  const char *colspace,
  const char *sort) {

  FILE *out;

  char file[LEN], quantity[LEN];

  int *cida, *ciqa, *cipa, *cira, *rida, *riqa, *ripa, *rira;

  size_t i, j, nc, nr;

  /* Check output flag... */
  if (!ctl->write_matrix)
    return;

  /* Allocate... */
  ALLOC(cida, int,
        M);
  ALLOC(ciqa, int,
        N);
  ALLOC(cipa, int,
        N);
  ALLOC(cira, int,
        M);
  ALLOC(rida, int,
        M);
  ALLOC(riqa, int,
        N);
  ALLOC(ripa, int,
        N);
  ALLOC(rira, int,
        M);

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write matrix: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

```

```
  /* Write header (row space)... */
  if (rowspace[0] == 'y') {

    fprintf(out,
            "# $1 = Row: index (measurement space)\n"
            "# $2 = Row: channel wavenumber [cm^-1]\n"
            "# $3 = Row: time (seconds since 2000-01-01T00:00Z)\n"
            "# $4 = Row: view point altitude [km]\n"
            "# $5 = Row: view point longitude [deg]\n"
            "# $6 = Row: view point latitude [deg]\n");

    /* Get number of rows... */
    nr = obs2y(ctl, obs, NULL, rida, rira);

  } else {

    fprintf(out,
            "# $1 = Row: index (state space)\n"
            "# $2 = Row: name of quantity\n"
            "# $3 = Row: time (seconds since 2000-01-01T00:00Z)\n"
            "# $4 = Row: altitude [km]\n"
            "# $5 = Row: longitude [deg]\n" "# $6 = Row: latitude [deg]\n");

    /* Get number of rows... */
    nr = atm2x(ctl, atm, NULL, riqa, ripa);
  }

  /* Write header (column space)... */
  if (colspace[0] == 'y') {

    fprintf(out,
            "# $7 = Col: index (measurement space)\n"
            "# $8 = Col: channel wavenumber [cm^-1]\n"
            "# $9 = Col: time (seconds since 2000-01-01T00:00Z)\n"
            "# $10 = Col: view point altitude [km]\n"
            "# $11 = Col: view point longitude [deg]\n"
            "# $12 = Col: view point latitude [deg]\n");

    /* Get number of columns... */
    nc = obs2y(ctl, obs, NULL, cida, cira);

  } else {

    fprintf(out,
            "# $7 = Col: index (state space)\n"
            "# $8 = Col: name of quantity\n"
            "# $9 = Col: time (seconds since 2000-01-01T00:00Z)\n"
            "# $10 = Col: altitude [km]\n"
            "# $11 = Col: longitude [deg]\n" "# $12 = Col: latitude [deg]\n");

    /* Get number of columns... */
    nc = atm2x(ctl, atm, NULL, ciqa, cipa);
  }

  /* Write header entry... */
  fprintf(out, "# $13 = Matrix element\n\n");

  /* Write matrix data... */
  i = j = 0;
  while (i < nr && j < nc) {

    /* Write info about the row... */
    if (rowspace[0] == 'y')
      fprintf(out, "%d %.4f %.2f %g %g %g",
              (int) i, ctl->nu[rida[i]],
              obs->time[rira[i]], obs->vpz[rira[i]],
              obs->vplon[rira[i]], obs->vplat[rira[i]]);
    else {
      idx2name(ctl, riqa[i], quantity);
      fprintf(out, "%d %s %.2f %g %g %g", (int) i, quantity,
              atm->time[ripa[i]], atm->z[ripa[i]],
              atm->lon[ripa[i]], atm->lat[ripa[i]]);
    }

    /* Write info about the column... */
    if (colspace[0] == 'y')
      fprintf(out, " %d %.4f %.2f %g %g %g",
              (int) j, ctl->nu[cida[j]],
              obs->time[cira[j]], obs->vpz[cira[j]],
              obs->vplon[cira[j]], obs->vplat[cira[j]]);
    else {
      idx2name(ctl, ciqa[j], quantity);
      fprintf(out, " %d %s %.2f %g %g %g", (int) j, quantity,
              atm->time[cipa[j]], atm->z[cipa[j]],
              atm->lon[cipa[j]], atm->lat[cipa[j]]);
    }

```

```
    /* Write matrix entry... */
    fprintf(out, " %g\n", gsl_matrix_get(matrix, i, j));

    /* Set matrix indices... */
    if (sort[0] == 'r') {
      j++;
      if (j >= nc) {
        j = 0;
        i++;
        fprintf(out, "\n");
      }
    } else {
      i++;
      if (i >= nr) {
        i = 0;
        j++;
        fprintf(out, "\n");
      }
    }
  }

  /* Close file... */
  fclose(out);

  /* Free... */
  free(cida);
  free(ciqa);
  free(cipa);
  free(cira);
  free(rida);
  free(riqa);
  free(ripa);
  free(rira);
}

/*****************************************************************************/

void write_obs(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  obs_t * obs) {

  FILE *out;

  char file[LEN];

  int n = 10;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write observation data: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n");
  for (int id = 0; id < ctl->nd; id++)
    fprintf(out, "# $%d = radiance (%.4f cm^-1) [W/(m^2 sr cm^-1)]\n",
            ++n, ctl->nu[id]);
  for (int id = 0; id < ctl->nd; id++)
    fprintf(out, "# $%d = transmittance (%.4f cm^-1) [-]\n", ++n,
            ctl->nu[id]);

  /* Write data... */
  for (int ir = 0; ir < obs->nr; ir++) {
    if (ir == 0 || obs->time[ir] != obs->time[ir - 1])
      fprintf(out, "\n");
    fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g", obs->time[ir],
            obs->obsz[ir], obs->obslon[ir], obs->obslat[ir],
```

```
          obs->vpz[ir], obs->vplon[ir], obs->vplat[ir],
          obs->tpz[ir], obs->tplon[ir], obs->tplat[ir]);
    for (int id = 0; id < ctl->nd; id++)
      fprintf(out, " %g", obs->rad[id][ir]);
    for (int id = 0; id < ctl->nd; id++)
      fprintf(out, " %g", obs->tau[id][ir]);
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);
}

/*****************************************************************************/

void write_shape(
  const char *filename,
  double *x,
  double *y,
  int n) {

  FILE *out;

  /* Write info... */
  LOG(1, "Write shape function: %s", filename);

  /* Create file... */
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = shape function x-value [-]\n"
          "# $2 = shape function y-value [-]\n\n");

  /* Write data... */
  for (int i = 0; i < n; i++)
    fprintf(out, "%.10g %.10g\n", x[i], y[i]);

  /* Close file... */
  fclose(out);
}

/*****************************************************************************/

void write_tbl(
  ctl_t * ctl,
  tbl_t * tbl) {

  FILE *out;

  char filename[2 * LEN];

  /* Loop over emitters and detectors... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int id = 0; id < ctl->nd; id++) {

      /* Set filename... */
      sprintf(filename, "%s_%.4f_%s.%s", ctl->tblbase,
              ctl->nu[id], ctl->emitter[ig],
              ctl->tblfmt == 1 ? "tab" : "bin");

      /* Write info... */
      LOG(1, "Write emissivity table: %s", filename);

      /* Create file... */
      if (!(out = fopen(filename, "w")))
        ERRMSG("Cannot create file!");

      /* Write ASCII data... */
      if (ctl->tblfmt == 1) {

        /* Write header... */
        fprintf(out,
                "# $1 = pressure [hPa]\n"
                "# $2 = temperature [K]\n"
                "# $3 = column density [molecules/cm^2]\n"
                "# $4 = emissivity [-]\n");

        /* Save table file... */
        for (int ip = 0; ip < tbl->np[id][ig]; ip++)
          for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
            fprintf(out, "\n");
            for (int iu = 0; iu < tbl->nu[id][ig][ip][it]; iu++)
              fprintf(out, "%g %g %e %e\n",
                      tbl->p[id][ig][ip], tbl->t[id][ig][ip][it],
                      tbl->u[id][ig][ip][it][iu],
```

```
                        tbl->eps[id][ig][ip][it][iu]);
            }
        }

        /* Write binary data... */
        else if (ctl->tblfmt == 2) {
          FWRITE(&tbl->np[id][ig], int,
                 1,
                 out);
          FWRITE(tbl->p[id][ig], double,
                   (size_t) tbl->np[id][ig],
                 out);
          for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
            FWRITE(&tbl->nt[id][ig][ip], int,
                   1,
                   out);
            FWRITE(tbl->t[id][ig][ip], double,
                     (size_t) tbl->nt[id][ig][ip],
                   out);
            for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
              FWRITE(&tbl->nu[id][ig][ip][it], int,
                     1,
                     out);
              FWRITE(tbl->u[id][ig][ip][it], float,
                       (size_t) tbl->nu[id][ig][ip][it],
                     out);
              FWRITE(tbl->eps[id][ig][ip][it], float,
                       (size_t) tbl->nu[id][ig][ip][it],
                     out);
            }
          }
        }

        /* Error message... */
        else
          ERRMSG("Unknown look-up table format!");

        /* Close file... */
        fclose(out);
      }
}

/*****************************************************************************/

void x2atm(
  ctl_t * ctl,
  gsl_vector * x,
  atm_t * atm) {

  size_t n = 0;

  /* Get pressure... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->retp_zmin && atm->z[ip] <= ctl->retp_zmax)
      x2atm_help(&atm->p[ip], x, &n);

  /* Get temperature... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->rett_zmin && atm->z[ip] <= ctl->rett_zmax)
      x2atm_help(&atm->t[ip], x, &n);

  /* Get volume mixing ratio... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retq_zmin[ig]
          && atm->z[ip] <= ctl->retq_zmax[ig])
        x2atm_help(&atm->q[ig][ip], x, &n);

  /* Get extinction... */
  for (int iw = 0; iw < ctl->nw; iw++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retk_zmin[iw]
          && atm->z[ip] <= ctl->retk_zmax[iw])
        x2atm_help(&atm->k[iw][ip], x, &n);

  /* Get cloud data... */
  if (ctl->ret_clz)
    x2atm_help(&atm->clz, x, &n);
  if (ctl->ret_cldz)
    x2atm_help(&atm->cldz, x, &n);
  if (ctl->ret_clk)
    for (int icl = 0; icl < ctl->ncl; icl++)
      x2atm_help(&atm->clk[icl], x, &n);

  /* Get surface data... */
  if (ctl->ret_sfz)
    x2atm_help(&atm->sfz, x, &n);
```

```
  if (ctl->ret_sfp)
    x2atm_help(&atm->sfp, x, &n);
  if (ctl->ret_sft)
    x2atm_help(&atm->sft, x, &n);
  if (ctl->ret_sfeps)
    for (int isf = 0; isf < ctl->nsf; isf++)
      x2atm_help(&atm->sfeps[isf], x, &n);
}

/*****************************************************************************/

void x2atm_help(
  double *value,
  gsl_vector * x,
  size_t *n) {

  /* Get state vector element... */
  *value = gsl_vector_get(x, *n);
  (*n)++;
}

/*****************************************************************************/

void y2obs(
  ctl_t * ctl,
  gsl_vector * y,
  obs_t * obs) {

  size_t m = 0;

  /* Decompose measurement vector... */
  for (int ir = 0; ir < obs->nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      if (gsl_finite(obs->rad[id][ir])) {
        obs->rad[id][ir] = gsl_vector_get(y, m);
        m++;
      }
}
```

5.19 jurassic.h File Reference

JURASSIC library declarations.

```
#include <gsl/gsl_math.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_linalg.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_statistics.h>
#include <math.h>
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <time.h>
```

Data Structures

- struct atm_t

    Atmospheric data.
- struct ctl_t

    Forward model control parameters.
- struct los_t

    Line-of-sight data.
- struct obs_t

    Observation geometry and radiance data.
- struct tbl_t

    Emissivity look-up tables.

Macros

- #define ALLOC(ptr, type, n)

  Allocate memory.
- #define DIST(a, b) sqrt(DIST2(a, b))

  Compute Cartesian distance between two vectors.
- #define DIST2(a, b) ((a[0]-b[0])∗(a[0]-b[0])+(a[1]-b[1])∗(a[1]-b[1])+(a[2]-b[2])∗(a[2]-b[2]))

  Compute squared distance between two vectors.
- #define DOTP(a, b) (a[0]∗b[0]+a[1]∗b[1]+a[2]∗b[2])

  Compute dot product of two vectors.
- #define EXP(x0, y0, x1, y1, x)

  Compute exponential interpolation.
- #define FREAD(ptr, type, size, out)

  Read binary data.
- #define FWRITE(ptr, type, size, out)

  Write binary data.
- #define LIN(x0, y0, x1, y1, x) ((y0)+((y1)-(y0))/((x1)-(x0))∗((x)-(x0)))

  Compute linear interpolation.
- #define NORM(a) sqrt(DOTP(a, a))

  Compute norm of a vector.
- #define POW2(x) ((x)∗(x))

  Compute x^2.
- #define POW3(x) ((x)∗(x)∗(x))

  Compute x^3.
- #define TIMER(name, mode) {timer(name, __FILE__, __func__, __LINE__, mode);}

  Start or stop a timer.
- #define TOK(line, tok, format, var)

  Read string tokens.
- #define LOGLEV 2

  Level of log messages (0=none, 1=basic, 2=detailed, 3=debug).
- #define LOG(level, ...)

  Print log message.
- #define WARN(...)

  Print warning message.
- #define ERRMSG(...)

  Print error message and quit program.
- #define PRINT(format, var)

  Print macro for debugging.
- #define TMIN 100.

  Minimum temperature for source function [K].
- #define TMAX 400.

  Maximum temperature for source function [K].
- #define TSUN 5780.

  Effective temperature of the sun [K].
- #define C1 1.19104259e-8

  First spectroscopic constant (c_1 = 2 h c^2) [W/(m^2 sr cm^-4)].
- #define C2 1.43877506

  Second spectroscopic constant (c_2 = h c / k) [K/cm^-1].
- #define G0 9.80665

  Standard gravity [m/s^2].
- #define KB 1.3806504e-23

Boltzmann constant [kg m^2/(K s^2)].

- #define NA 6.02214199e23

  Avogadro's number.

- #define H0 7.0

  Standard scale height [km].

- #define P0 1013.25

  Standard pressure [hPa].

- #define T0 273.15

  Standard temperature [K].

- #define RE 6367.421

  Mean radius of Earth [km].

- #define RI 8.3144598

  Ideal gas constant [J/(mol K)].

- #define ME 5.976e24

  Mass of Earth [kg].

- #define NCL 8

  Maximum number of cloud layer spectral grid points.

- #define ND 64

  Maximum number of radiance channels.

- #define NG 8

  Maximum number of emitters.

- #define NP 256

  Maximum number of atmospheric data points.

- #define NR 256

  Maximum number of ray paths.

- #define NSF 8

  Maximum number of surface layer spectral grid points.

- #define NW 4

  Maximum number of spectral windows.

- #define LEN 10000

  Maximum length of ASCII data lines.

- #define M (NR∗ND)

  Maximum size of measurement vector.

- #define N ((2+NG+NW)∗NP+NCL+NSF+5)

  Maximum size of state vector.

- #define NQ (7+NG+NW+NCL+NSF)

  Maximum number of quantities.

- #define NLOS 4096

  Maximum number of LOS points.

- #define NSHAPE 10000

  Maximum number of shape function grid points.

- #define NFOV 5

  Number of ray paths used for FOV calculations.

- #define TBLNP 41

  Maximum number of pressure levels in emissivity tables.

- #define TBLNT 30

  Maximum number of temperatures in emissivity tables.

- #define TBLNU 320

  Maximum number of column densities in emissivity tables.

- #define TBLNS 1200

  Maximum number of source function temperature levels.

- #define RFMNPTS 10000000

  Maximum number of RFM spectral grid points.
- #define RFMLINE 100000

  Maximum length of RFM data lines.
- #define IDXP 0

  Index for pressure.
- #define IDXT 1

  Index for temperature.
- #define IDXQ(ig) (2+ig)

  Indices for volume mixing ratios.
- #define IDXK(iw) (2+ctl->ng+iw)

  Indices for extinction.
- #define IDXCLZ (2+ctl->ng+ctl->nw)

  Index for cloud layer height.
- #define IDXCLDZ (3+ctl->ng+ctl->nw)

  Index for cloud layer depth.
- #define IDXCLK(icl) (4+ctl->ng+ctl->nw+icl)

  Indices for cloud layer extinction.
- #define IDXSFZ (4+ctl->ng+ctl->nw+ctl->ncl)

  Index for surface layer height.
- #define IDXSFP (5+ctl->ng+ctl->nw+ctl->ncl)

  Index for surface layer pressure.
- #define IDXSFT (6+ctl->ng+ctl->nw+ctl->ncl)

  Index for surface layer temperature.
- #define IDXSFEPS(isf) (7+ctl->ng+ctl->nw+ctl->ncl+isf)

  Indices for surface layer emissivity.

Functions

- size_t atm2x (ctl_t *ctl, atm_t *atm, gsl_vector *x, int *iqa, int *ipa)

  Compose state vector or parameter vector.
- void atm2x_help (double value, int value_iqa, int value_ip, gsl_vector *x, int *iqa, int *ipa, size_t *n)

  Add element to state vector.
- double brightness (double rad, double nu)

  Compute brightness temperature.
- void cart2geo (double *x, double *z, double *lon, double *lat)

  Convert Cartesian coordinates to geolocation.
- void climatology (ctl_t *ctl, atm_t *atm_mean)

  Interpolate climatological data.
- double ctmco2 (double nu, double p, double t, double u)

  Compute carbon dioxide continuum (optical depth).
- double ctmh2o (double nu, double p, double t, double q, double u)

  Compute water vapor continuum (optical depth).
- double ctmn2 (double nu, double p, double t)

  Compute nitrogen continuum (absorption coefficient).
- double ctmo2 (double nu, double p, double t)

  Compute oxygen continuum (absorption coefficient).
- void copy_atm (ctl_t *ctl, atm_t *atm_dest, atm_t *atm_src, int init)

  Copy and initialize atmospheric data.
- void copy_obs (ctl_t *ctl, obs_t *obs_dest, obs_t *obs_src, int init)

Copy and initialize observation data.
- int find_emitter (ctl_t ∗ctl, const char ∗emitter)

  Find index of an emitter.
- void formod (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs)

  Determine ray paths and compute radiative transfer.
- void formod_continua (ctl_t ∗ctl, los_t ∗los, int ip, double ∗beta)

  Compute absorption coefficient of continua.
- void formod_fov (ctl_t ∗ctl, obs_t ∗obs)

  Apply field of view convolution.
- void formod_pencil (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs, int ir)

  Compute radiative transfer for a pencil beam.
- void formod_rfm (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs)

  Apply RFM for radiative transfer calculations.
- void formod_srcfunc (ctl_t ∗ctl, tbl_t ∗tbl, double t, double ∗src)

  Compute Planck source function.
- void geo2cart (double z, double lon, double lat, double ∗x)

  Convert geolocation to Cartesian coordinates.
- void hydrostatic (ctl_t ∗ctl, atm_t ∗atm)

  Set hydrostatic equilibrium.
- void idx2name (ctl_t ∗ctl, int idx, char ∗quantity)

  Determine name of state vector quantity for given index.
- void init_srcfunc (ctl_t ∗ctl, tbl_t ∗tbl)

  Initialize source function table.
- void intpol_atm (ctl_t ∗ctl, atm_t ∗atm, double z, double ∗p, double ∗t, double ∗q, double ∗k)

  Interpolate atmospheric data.
- void intpol_tbl (ctl_t ∗ctl, tbl_t ∗tbl, los_t ∗los, int ip, double tau_path[ND][NG], double tau_seg[ND])

  Get transmittance from look-up tables.
- double intpol_tbl_eps (tbl_t ∗tbl, int ig, int id, int ip, int it, double u)

  Interpolate emissivity from look-up tables.
- double intpol_tbl_u (tbl_t ∗tbl, int ig, int id, int ip, int it, double eps)

  Interpolate column density from look-up tables.
- void jsec2time (double jsec, int ∗year, int ∗mon, int ∗day, int ∗hour, int ∗min, int ∗sec, double ∗remain)

  Convert seconds to date.
- void kernel (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs, gsl_matrix ∗k)

  Compute Jacobians.
- int locate_irr (double ∗xx, int n, double x)

  Find array index for irregular grid.
- int locate_reg (double ∗xx, int n, double x)

  Find array index for regular grid.
- int locate_tbl (float ∗xx, int n, double x)

  Find array index in float array.
- size_t obs2y (ctl_t ∗ctl, obs_t ∗obs, gsl_vector ∗y, int ∗ida, int ∗ira)

  Compose measurement vector.
- double planck (double t, double nu)

  Compute Planck function.
- void raytrace (ctl_t ∗ctl, atm_t ∗atm, obs_t ∗obs, los_t ∗los, int ir)

  Do ray-tracing to determine LOS.
- void read_atm (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, atm_t ∗atm)

  Read atmospheric data.
- void read_ctl (int argc, char ∗argv[ ], ctl_t ∗ctl)

  Read forward model control parameters.

- void read_matrix (const char ∗dirname, const char ∗filename, gsl_matrix ∗matrix)

    Read matrix.
- void read_obs (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, obs_t ∗obs)

    Read observation data.
- double read_obs_rfm (const char ∗basename, double z, double ∗nu, double ∗f, int n)

    Read observation data in RFM format.
- void read_rfm_spec (const char ∗filename, double ∗nu, double ∗rad, int ∗npts)

    Read RFM spectrum.
- void read_shape (const char ∗filename, double ∗x, double ∗y, int ∗n)

    Read shape function.
- void read_tbl (ctl_t ∗ctl, tbl_t ∗tbl)

    Read look-up table data.
- double refractivity (double p, double t)

    Compute refractivity (return value is n - 1).
- double scan_ctl (int argc, char ∗argv[ ], const char ∗varname, int arridx, const char ∗defvalue, char ∗value)

    Search control parameter file for variable entry.
- double sza (double sec, double lon, double lat)

    Calculate solar zenith angle.
- void tangent_point (los_t ∗los, double ∗tpz, double ∗tplon, double ∗tplat)

    Find tangent point of a given LOS.
- void time2jsec (int year, int mon, int day, int hour, int min, int sec, double remain, double ∗jsec)

    Convert date to seconds.
- void timer (const char ∗name, const char ∗file, const char ∗func, int line, int mode)

    Measure wall-clock time.
- void write_atm (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, atm_t ∗atm)

    Write atmospheric data.
- void write_atm_rfm (const char ∗filename, ctl_t ∗ctl, atm_t ∗atm)

    Write atmospheric data in RFM format.
- void write_matrix (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, gsl_matrix ∗matrix, atm_t ∗atm, obs_t ∗obs, const char ∗rowspace, const char ∗colspace, const char ∗sort)

    Write matrix.
- void write_obs (const char ∗dirname, const char ∗filename, ctl_t ∗ctl, obs_t ∗obs)

    Write observation data.
- void write_shape (const char ∗filename, double ∗x, double ∗y, int n)

    Write shape function.
- void write_tbl (ctl_t ∗ctl, tbl_t ∗tbl)

    Write look-up table data.
- void x2atm (ctl_t ∗ctl, gsl_vector ∗x, atm_t ∗atm)

    Decompose parameter vector or state vector.
- void x2atm_help (double ∗value, gsl_vector ∗x, size_t ∗n)

    Get element from state vector.
- void y2obs (ctl_t ∗ctl, gsl_vector ∗y, obs_t ∗obs)

    Decompose measurement vector.

5.19.1 Detailed Description

JURASSIC library declarations.

Definition in file jurassic.h.

5.19.2 Macro Definition Documentation

5.19.2.1 ALLOC

```
#define ALLOC(
    ptr,
    type,
    n )
```

Value:

```
if((ptr=malloc((size_t)(n)*sizeof(type)))==NULL)       \
  ERRMSG("Out of memory!");
```

Allocate memory.

Definition at line 58 of file jurassic.h.

5.19.2.2 DIST

```
#define DIST(
    a,
    b ) sqrt(DIST2(a, b))
```

Compute Cartesian distance between two vectors.

Definition at line 63 of file jurassic.h.

5.19.2.3 DIST2

```
#define DIST2(
    a,
    b )   ((a[0]-b[0])*(a[0]-b[0])+(a[1]-b[1])*(a[1]-b[1])+(a[2]-b[2])*(a[2]-b[2]))
```

Compute squared distance between two vectors.

Definition at line 66 of file jurassic.h.

5.19.2.4 DOTP

```
#define DOTP(
    a,
    b ) (a[0]*b[0]+a[1]*b[1]+a[2]*b[2])
```

Compute dot product of two vectors.

Definition at line 70 of file jurassic.h.

5.19.2.5 EXP

```
#define EXP(
    x0,
    y0,
    x1,
    y1,
    x )
```

Value:

```
(((y0)>0 && (y1)>0)                                              \
 ? ((y0)*exp(log((y1)/(y0))/((x1)-(x0))*((x)-(x0))))             \
 : LIN(x0, y0, x1, y1, x))
```

Compute exponential interpolation.

Definition at line 73 of file jurassic.h.

5.19.2.6 FREAD

```
#define FREAD(
    ptr,
    type,
    size,
    out )
```

Value:

```
  {                                     \
  if(fread(ptr, sizeof(type), size, out)!=size)                  \
    ERRMSG("Error while reading!");                              \
}
```

Read binary data.

Definition at line 79 of file jurassic.h.

5.19.2.7 FWRITE

```
#define FWRITE(
    ptr,
    type,
    size,
    out )
```

Value:

```
  {                                     \
  if(fwrite(ptr, sizeof(type), size, out)!=size)                 \
    ERRMSG("Error while writing!");                              \
}
```

Write binary data.

Definition at line 85 of file jurassic.h.

5.19.2.8 LIN

```
#define LIN(
    x0,
    y0,
    x1,
    y1,
    x ) ((y0)+((y1)-(y0))/((x1)-(x0))*((x)-(x0)))
```

Compute linear interpolation.

Definition at line 91 of file jurassic.h.

5.19.2.9 NORM

```
#define NORM(
    a ) sqrt(DOTP(a, a))
```

Compute norm of a vector.

Definition at line 95 of file jurassic.h.

5.19.2.10 POW2

```
#define POW2(
    x ) ((x)*(x))
```

Compute x^2.

Definition at line 98 of file jurassic.h.

5.19.2.11 POW3

```
#define POW3(
    x ) ((x)*(x)*(x))
```

Compute x^3.

Definition at line 101 of file jurassic.h.

5.19.2.12 TIMER

```
#define TIMER(
    name,
    mode ) {timer(name, __FILE__, __func__, __LINE__, mode);}
```

Start or stop a timer.

Definition at line 104 of file jurassic.h.

5.19.2.13 TOK

```
#define TOK(
    line,
    tok,
    format,
    var )
```

Value:

```
{                              \
    if(((tok)=strtok((line), " \t"))) {            \
      if(sscanf(tok, format, &(var))!=1) continue;      \
    } else ERRMSG("Error while reading!");           \
  }
```

Read string tokens.

Definition at line 108 of file jurassic.h.

5.19.2.14 LOGLEV

```
#define LOGLEV 2
```

Level of log messages (0=none, 1=basic, 2=detailed, 3=debug).

Definition at line 120 of file jurassic.h.

5.19.2.15 LOG

```
#define LOG(
    level,
    ... )
```

Value:

```
{                                       \
    if(level >= 2)                                  \
      printf("  ");                                 \
    if(level <= LOGLEV) {                        \
      printf(__VA_ARGS__);                          \
      printf("\n");                                 \
    }                                               \
  }
```

Print log message.

Definition at line 124 of file jurassic.h.

5.19.2.16 WARN

```
#define WARN(
    ... )
```

Value:

```
{                                           \
    printf("\nWarning (%s, %s, l%d): ", __FILE__, __func__, __LINE__);  \
    LOG(0, __VA_ARGS__);                                  \
  }
```

Print warning message.

Definition at line 134 of file jurassic.h.

5.19.2.17 ERRMSG

```
#define ERRMSG(
    ... )
```

Value:

```
{                                                             \
    printf("\nError (%s, %s, l%d): ", __FILE__, __func__, __LINE__);    \
    LOG(0, __VA_ARGS__);                                                \
    exit(EXIT_FAILURE);                                                 \
  }
```

Print error message and quit program.

Definition at line 140 of file jurassic.h.

5.19.2.18 PRINT

```
#define PRINT(
    format,
    var )
```

Value:

```
printf("Print (%s, %s, l%d): %s= "format"\n",                          \
       __FILE__, __func__, __LINE__, #var, var);
```

Print macro for debugging.

Definition at line 147 of file jurassic.h.

5.19.2.19 TMIN

```
#define TMIN 100.
```

Minimum temperature for source function [K].

Definition at line 156 of file jurassic.h.

5.19.2.20 TMAX

```
#define TMAX 400.
```

Maximum temperature for source function [K].

Definition at line 159 of file jurassic.h.

5.19.2.21 TSUN

```
#define TSUN 5780.
```

Effective temperature of the sun [K].

Definition at line 162 of file jurassic.h.

5.19.2.22 C1 `#define C1 1.19104259e-8`

First spectroscopic constant (c_1 = 2 h c^2) [W/(m^2 sr cm^-4)].

Definition at line 165 of file jurassic.h.

5.19.2.23 C2 `#define C2 1.43877506`

Second spectroscopic constant (c_2 = h c / k) [K/cm^-1].

Definition at line 168 of file jurassic.h.

5.19.2.24 G0 `#define G0 9.80665`

Standard gravity [m/s^2].

Definition at line 171 of file jurassic.h.

5.19.2.25 KB `#define KB 1.3806504e-23`

Boltzmann constant [kg m^2/(K s^2)].

Definition at line 174 of file jurassic.h.

5.19.2.26 NA `#define NA 6.02214199e23`

Avogadro's number.

Definition at line 177 of file jurassic.h.

5.19.2.27 H0 `#define H0 7.0`

Standard scale height [km].

Definition at line 180 of file jurassic.h.

5.19.2.28 P0 `#define P0 1013.25`

Standard pressure [hPa].

Definition at line 183 of file jurassic.h.

5.19.2.29 T0 `#define T0 273.15`

Standard temperature [K].

Definition at line 186 of file jurassic.h.

5.19.2.30 RE `#define RE 6367.421`

Mean radius of Earth [km].

Definition at line 189 of file jurassic.h.

5.19.2.31 RI `#define RI 8.3144598`

Ideal gas constant [J/(mol K)].

Definition at line 192 of file jurassic.h.

5.19.2.32 ME `#define ME 5.976e24`

Mass of Earth [kg].

Definition at line 195 of file jurassic.h.

5.19.2.33 NCL `#define NCL 8`

Maximum number of cloud layer spectral grid points.

Definition at line 203 of file jurassic.h.

5.19.2.34 ND `#define ND 64`

Maximum number of radiance channels.

Definition at line 208 of file jurassic.h.

5.19.2.35 NG `#define NG 8`

Maximum number of emitters.

Definition at line 213 of file jurassic.h.

5.19.2.36 NP `#define NP 256`

Maximum number of atmospheric data points.

Definition at line 218 of file jurassic.h.

5.19.2.37 NR `#define NR 256`

Maximum number of ray paths.

Definition at line 223 of file jurassic.h.

5.19.2.38 NSF `#define NSF 8`

Maximum number of surface layer spectral grid points.

Definition at line 228 of file jurassic.h.

5.19.2.39 NW `#define NW 4`

Maximum number of spectral windows.

Definition at line 233 of file jurassic.h.

5.19.2.40 LEN `#define LEN 10000`

Maximum length of ASCII data lines.

Definition at line 238 of file jurassic.h.

5.19.2.41 M `#define M (NR*ND)`

Maximum size of measurement vector.

Definition at line 243 of file jurassic.h.

5.19.2.42 N `#define N ((2+NG+NW)*NP+NCL+NSF+5)`

Maximum size of state vector.

Definition at line 248 of file jurassic.h.

5.19.2.43 NQ `#define NQ (7+NG+NW+NCL+NSF)`

Maximum number of quantities.

Definition at line 253 of file jurassic.h.

5.19.2.44 NLOS `#define NLOS 4096`

Maximum number of LOS points.

Definition at line 258 of file jurassic.h.

5.19.2.45 NSHAPE `#define NSHAPE 10000`

Maximum number of shape function grid points.

Definition at line 263 of file jurassic.h.

5.19.2.46 NFOV `#define NFOV 5`

Number of ray paths used for FOV calculations.

Definition at line 268 of file jurassic.h.

5.19.2.47 TBLNP `#define TBLNP 41`

Maximum number of pressure levels in emissivity tables.

Definition at line 273 of file jurassic.h.

5.19.2.48 TBLNT `#define TBLNT 30`

Maximum number of temperatures in emissivity tables.

Definition at line 278 of file jurassic.h.

5.19.2.49 TBLNU `#define TBLNU 320`

Maximum number of column densities in emissivity tables.

Definition at line 283 of file jurassic.h.

5.19.2.50 TBLNS `#define TBLNS 1200`

Maximum number of source function temperature levels.

Definition at line 288 of file jurassic.h.

5.19.2.51 RFMNPTS `#define RFMNPTS 10000000`

Maximum number of RFM spectral grid points.

Definition at line 293 of file jurassic.h.

5.19.2.52 RFMLINE `#define RFMLINE 100000`

Maximum length of RFM data lines.

Definition at line 298 of file jurassic.h.

5.19.2.53 IDXP `#define IDXP 0`

Index for pressure.

Definition at line 306 of file jurassic.h.

5.19.2.54 IDXT `#define IDXT 1`

Index for temperature.

Definition at line 309 of file jurassic.h.

5.19.2.55 IDXQ `#define IDXQ( ig ) (2+ig)`

Indices for volume mixing ratios.

Definition at line 312 of file jurassic.h.

5.19.2.56 IDXK `#define IDXK( iw ) (2+ctl->ng+iw)`

Indices for extinction.

Definition at line 315 of file jurassic.h.

5.19.2.57 IDXCLZ `#define IDXCLZ (2+ctl->ng+ctl->nw)`

Index for cloud layer height.

Definition at line 318 of file jurassic.h.

5.19.2.58 IDXCLDZ `#define IDXCLDZ (3+ctl->ng+ctl->nw)`

Index for cloud layer depth.

Definition at line 321 of file jurassic.h.

5.19.2.59 IDXCLK `#define IDXCLK( icl ) (4+ctl->ng+ctl->nw+icl)`

Indices for cloud layer extinction.

Definition at line 324 of file jurassic.h.

5.19.2.60 IDXSFZ `#define IDXSFZ (4+ctl->ng+ctl->nw+ctl->ncl)`

Index for surface layer height.

Definition at line 327 of file jurassic.h.

5.19.2.61 IDXSFP `#define IDXSFP (5+ctl->ng+ctl->nw+ctl->ncl)`

Index for surface layer pressure.

Definition at line 330 of file jurassic.h.

5.19.2.62 IDXSFT `#define IDXSFT (6+ctl->ng+ctl->nw+ctl->ncl)`

Index for surface layer temperature.

Definition at line 333 of file jurassic.h.

5.19.2.63 IDXSFEPS `#define IDXSFEPS( isf ) (7+ctl->ng+ctl->nw+ctl->ncl+isf)`

Indices for surface layer emissivity.

Definition at line 336 of file jurassic.h.

5.19.3 Function Documentation

5.19.3.1 atm2x()

```
size_t atm2x (
        ctl_t * ctl,
        atm_t * atm,
        gsl_vector * x,
        int * iqa,
        int * ipa )
```

Compose state vector or parameter vector.

Definition at line 29 of file jurassic.c.

```
                 {

  size_t n = 0;

  /* Add pressure... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->retp_zmin && atm->z[ip] <= ctl->retp_zmax)
      atm2x_help(atm->p[ip], IDXP, ip, x, iqa, ipa, &n);

  /* Add temperature... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->rett_zmin && atm->z[ip] <= ctl->rett_zmax)
      atm2x_help(atm->t[ip], IDXT, ip, x, iqa, ipa, &n);

  /* Add volume mixing ratios... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retq_zmin[ig]
          && atm->z[ip] <= ctl->retq_zmax[ig])
        atm2x_help(atm->q[ig][ip], IDXQ(ig), ip, x, iqa, ipa, &n);

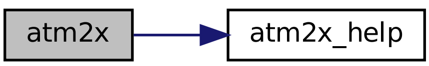
  /* Add extinction... */
  for (int iw = 0; iw < ctl->nw; iw++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retk_zmin[iw]
          && atm->z[ip] <= ctl->retk_zmax[iw])
        atm2x_help(atm->k[iw][ip], IDXK(iw), ip, x, iqa, ipa, &n);

  /* Add cloud parameters... */
  if (ctl->ret_clz)
    atm2x_help(atm->clz, IDXCLZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_cldz)
    atm2x_help(atm->cldz, IDXCLDZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_clk)
    for (int icl = 0; icl < ctl->ncl; icl++)
      atm2x_help(atm->clk[icl], IDXCLK(icl), 0, x, iqa, ipa, &n);

  /* Add surface parameters... */
  if (ctl->ret_sfz)
    atm2x_help(atm->sfz, IDXSFZ, 0, x, iqa, ipa, &n);
  if (ctl->ret_sfp)
    atm2x_help(atm->sfp, IDXSFP, 0, x, iqa, ipa, &n);
  if (ctl->ret_sft)
    atm2x_help(atm->sft, IDXSFT, 0, x, iqa, ipa, &n);
  if (ctl->ret_sfeps)
    for (int isf = 0; isf < ctl->nsf; isf++)
      atm2x_help(atm->sfeps[isf], IDXSFEPS(isf), 0, x, iqa, ipa, &n);

  return n;
}
```

Here is the call graph for this function:



5.19.3.2 atm2x_help()

```
void atm2x_help (
        double value,
        int value_iqa,
        int value_ip,
        gsl_vector * x,
        int * iqa,
        int * ipa,
        size_t * n )
```

Add element to state vector.

Definition at line 87 of file jurassic.c.

```
                 {

  /* Add element to state vector... */
  if (x != NULL)
    gsl_vector_set(x, *n, value);
  if (iqa != NULL)
    iqa[*n] = value_iqa;
  if (ipa != NULL)
    ipa[*n] = value_ip;
  (*n)++;
}
```

5.19.3.3 brightness()

```
double brightness (
        double rad,
        double nu )
```

Compute brightness temperature.

Definition at line 109 of file jurassic.c.

```
                 {

  return C2 * nu / gsl_log1p(C1 * POW3(nu) / rad);
}
```

5.19.3.4 cart2geo()

```
void cart2geo (
        double * x,
        double * z,
        double * lon,
        double * lat )
```

Convert Cartesian coordinates to geolocation.

Definition at line 119 of file jurassic.c.

```
                   {

  double radius = NORM(x);

  *lat = asin(x[2] / radius) * 180 / M_PI;
  *lon = atan2(x[1], x[0]) * 180 / M_PI;
  *z = radius - RE;
}
```

5.19.3.5 climatology()

```
void climatology (
        ctl_t * ctl,
        atm_t * atm_mean )
```

Interpolate climatological data.

Definition at line 134 of file jurassic.c.

```
                 {

  static double z[121] = {
    0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,
    20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37,
    38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55,
    56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73,
    74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91,
    92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107,
    108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120
  };

  static double pre[121] = {
    1017, 901.083, 796.45, 702.227, 617.614, 541.644, 473.437, 412.288,
    357.603, 308.96, 265.994, 228.348, 195.619, 167.351, 143.039, 122.198,
    104.369, 89.141, 76.1528, 65.0804, 55.641, 47.591, 40.7233, 34.8637,
    29.8633, 25.5956, 21.9534, 18.8445, 16.1909, 13.9258, 11.9913,
    10.34, 8.92988, 7.72454, 6.6924, 5.80701, 5.04654, 4.39238, 3.82902,
    3.34337, 2.92413, 2.56128, 2.2464, 1.97258, 1.73384, 1.52519, 1.34242,
    1.18197, 1.04086, 0.916546, 0.806832, 0.709875, 0.624101, 0.548176,
    0.480974, 0.421507, 0.368904, 0.322408, 0.281386, 0.245249, 0.213465,
    0.185549, 0.161072, 0.139644, 0.120913, 0.104568, 0.0903249, 0.0779269,
    0.0671493, 0.0577962, 0.0496902, 0.0426736, 0.0366093, 0.0313743,
    0.0268598, 0.0229699, 0.0196206, 0.0167399, 0.0142646, 0.0121397,
    0.0103181, 0.00875775, 0.00742226, 0.00628076, 0.00530519, 0.00447183,
    0.00376124, 0.00315632, 0.00264248, 0.00220738, 0.00184003, 0.00153095,
    0.00127204, 0.00105608, 0.000876652, 0.00072798, 0.00060492,
    0.000503201, 0.000419226, 0.000349896, 0.000292659, 0.000245421,
    0.000206394, 0.000174125, 0.000147441, 0.000125333, 0.000106985,
    9.173e-05, 7.90172e-05, 6.84172e-05, 5.95574e-05, 5.21183e-05,
    4.58348e-05, 4.05127e-05, 3.59987e-05, 3.21583e-05, 2.88718e-05,
    2.60322e-05, 2.35687e-05, 2.14263e-05, 1.95489e-05
  };

  static double tem[121] = {
    285.14, 279.34, 273.91, 268.3, 263.24, 256.55, 250.2, 242.82, 236.17,
    229.87, 225.04, 221.19, 218.85, 217.19, 216.2, 215.68, 215.42, 215.55,
    215.92, 216.4, 216.93, 217.45, 218, 218.68, 219.39, 220.25, 221.3,
    222.41, 223.88, 225.42, 227.2, 229.52, 231.89, 234.51, 236.85, 239.42,
    241.94, 244.57, 247.36, 250.32, 253.34, 255.82, 258.27, 260.39,
    262.03, 263.45, 264.2, 264.78, 264.67, 264.38, 263.24, 262.03, 260.02,
    258.09, 255.63, 253.28, 250.43, 247.81, 245.26, 242.77, 240.38,
    237.94, 235.79, 233.53, 231.5, 229.53, 227.6, 225.62, 223.77, 222.06,
    220.33, 218.69, 217.18, 215.64, 214.13, 212.52, 210.86, 209.25,
    207.49, 205.81, 204.11, 202.22, 200.32, 198.39, 195.92, 193.46,
    190.94, 188.31, 185.82, 183.57, 181.43, 179.74, 178.64, 178.1, 178.25,
    178.7, 179.41, 180.67, 182.31, 184.18, 186.6, 189.53, 192.66, 196.54,
    201.13, 205.93, 211.73, 217.86, 225, 233.53, 242.57, 252.14, 261.48,
    272.97, 285.26, 299.12, 312.2, 324.17, 338.34, 352.56, 365.28
  };

  static double c2h2[121] = {
    1.352e-09, 2.83e-10, 1.269e-10, 6.926e-11, 4.346e-11, 2.909e-11,
    2.014e-11, 1.363e-11, 8.71e-12, 5.237e-12, 2.718e-12, 1.375e-12,
    5.786e-13, 2.16e-13, 7.317e-14, 2.551e-14, 1.055e-14, 4.758e-15,
    2.056e-15, 7.703e-16, 2.82e-16, 1.035e-16, 4.382e-17, 1.946e-17,
    9.638e-18, 5.2e-18, 2.811e-18, 1.494e-18, 7.925e-19, 4.213e-19,
    1.998e-19, 8.78e-20, 3.877e-20, 1.728e-20, 7.743e-21, 3.536e-21,
    1.623e-21, 7.508e-22, 3.508e-22, 1.65e-22, 7.837e-23, 3.733e-23,
    1.808e-23, 8.77e-24, 4.285e-24, 2.095e-24, 1.032e-24, 5.082e-25,
    2.506e-25, 1.236e-25, 6.088e-26, 2.996e-26, 1.465e-26, 0, 0, 0,
    0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
    0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
    0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
  };

  static double c2h6[121] = {
    2.667e-09, 2.02e-09, 1.658e-09, 1.404e-09, 1.234e-09, 1.109e-09,
    1.012e-09, 9.262e-10, 8.472e-10, 7.71e-10, 6.932e-10, 6.216e-10,
    5.503e-10, 4.87e-10, 4.342e-10, 3.861e-10, 3.347e-10, 2.772e-10,
    2.209e-10, 1.672e-10, 1.197e-10, 8.536e-11, 5.783e-11, 3.846e-11,
    2.495e-11, 1.592e-11, 1.017e-11, 6.327e-12, 3.895e-12, 2.403e-12,
    1.416e-12, 8.101e-13, 4.649e-13, 2.686e-13, 1.557e-13, 9.14e-14,
    5.386e-14, 3.19e-14, 1.903e-14, 1.14e-14, 6.875e-15, 4.154e-15,
    2.538e-15, 1.553e-15, 9.548e-16, 5.872e-16, 3.63e-16, 2.244e-16,
    1.388e-16, 8.587e-17, 5.308e-17, 3.279e-17, 2.017e-17, 1.238e-17,
    7.542e-18, 4.585e-18, 2.776e-18, 1.671e-18, 9.985e-19, 5.937e-19,
```

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    3.518e-19, 2.07e-19, 1.215e-19, 7.06e-20, 4.097e-20, 2.37e-20,
    1.363e-20, 7.802e-21, 4.441e-21, 2.523e-21, 1.424e-21, 8.015e-22,
    4.497e-22, 2.505e-22, 1.391e-22, 7.691e-23, 4.238e-23, 2.331e-23,
    1.274e-23, 6.929e-24, 3.752e-24, 2.02e-24, 1.083e-24, 5.774e-25,
    3.041e-25, 1.593e-25, 8.308e-26, 4.299e-26, 2.195e-26, 1.112e-26,
    0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
    0, 0, 0, 0, 0, 0, 0, 0, 0
  };

  static double ccl4[121] = {
    1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10, 1.075e-10,
    1.075e-10, 1.075e-10, 1.075e-10, 1.06e-10, 1.024e-10, 9.69e-11,
    8.93e-11, 8.078e-11, 7.213e-11, 6.307e-11, 5.383e-11, 4.49e-11,
    3.609e-11, 2.705e-11, 1.935e-11, 1.385e-11, 8.35e-12, 5.485e-12,
    3.853e-12, 2.22e-12, 5.875e-13, 3.445e-13, 1.015e-13, 6.075e-14,
    4.383e-14, 2.692e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14, 1e-14,
    1e-14, 1e-14, 1e-14
  };

  static double ch4[121] = {
    1.864e-06, 1.835e-06, 1.819e-06, 1.805e-06, 1.796e-06, 1.788e-06,
    1.782e-06, 1.776e-06, 1.769e-06, 1.761e-06, 1.749e-06, 1.734e-06,
    1.716e-06, 1.692e-06, 1.654e-06, 1.61e-06, 1.567e-06, 1.502e-06,
    1.433e-06, 1.371e-06, 1.323e-06, 1.277e-06, 1.232e-06, 1.188e-06,
    1.147e-06, 1.108e-06, 1.07e-06, 1.027e-06, 9.854e-07, 9.416e-07,
    8.933e-07, 8.478e-07, 7.988e-07, 7.515e-07, 7.07e-07, 6.64e-07,
    6.239e-07, 5.864e-07, 5.512e-07, 5.184e-07, 4.87e-07, 4.571e-07,
    4.296e-07, 4.04e-07, 3.802e-07, 3.578e-07, 3.383e-07, 3.203e-07,
    3.032e-07, 2.889e-07, 2.76e-07, 2.635e-07, 2.519e-07, 2.409e-07,
    2.302e-07, 2.219e-07, 2.144e-07, 2.071e-07, 1.999e-07, 1.93e-07,
    1.862e-07, 1.795e-07, 1.731e-07, 1.668e-07, 1.607e-07, 1.548e-07,
    1.49e-07, 1.434e-07, 1.38e-07, 1.328e-07, 1.277e-07, 1.227e-07,
    1.18e-07, 1.134e-07, 1.089e-07, 1.046e-07, 1.004e-07, 9.635e-08,
    9.245e-08, 8.867e-08, 8.502e-08, 8.15e-08, 7.809e-08, 7.48e-08,
    7.159e-08, 6.849e-08, 6.55e-08, 6.262e-08, 5.98e-08, 5.708e-08,
    5.448e-08, 5.194e-08, 4.951e-08, 4.72e-08, 4.5e-08, 4.291e-08,
    4.093e-08, 3.905e-08, 3.729e-08, 3.563e-08, 3.408e-08, 3.265e-08,
    3.128e-08, 2.996e-08, 2.87e-08, 2.76e-08, 2.657e-08, 2.558e-08,
    2.467e-08, 2.385e-08, 2.307e-08, 2.234e-08, 2.168e-08, 2.108e-08,
    2.05e-08, 1.998e-08, 1.947e-08, 1.902e-08, 1.86e-08, 1.819e-08,
    1.782e-08
  };

  static double clo[121] = {
    7.419e-15, 1.061e-14, 1.518e-14, 2.195e-14, 3.175e-14, 4.666e-14,
    6.872e-14, 1.03e-13, 1.553e-13, 2.375e-13, 3.664e-13, 5.684e-13,
    8.915e-13, 1.402e-12, 2.269e-12, 4.125e-12, 7.501e-12, 1.257e-11,
    2.048e-11, 3.338e-11, 5.44e-11, 8.846e-11, 1.008e-10, 1.082e-10,
    1.157e-10, 1.232e-10, 1.312e-10, 1.539e-10, 1.822e-10, 2.118e-10,
    2.387e-10, 2.687e-10, 2.875e-10, 3.031e-10, 3.23e-10, 3.648e-10,
    4.117e-10, 4.477e-10, 4.633e-10, 4.794e-10, 4.95e-10, 5.104e-10,
    5.259e-10, 5.062e-10, 4.742e-10, 4.443e-10, 4.051e-10, 3.659e-10,
    3.305e-10, 2.911e-10, 2.54e-10, 2.215e-10, 1.927e-10, 1.675e-10,
    1.452e-10, 1.259e-10, 1.09e-10, 9.416e-11, 8.119e-11, 6.991e-11,
    6.015e-11, 5.163e-11, 4.43e-11, 3.789e-11, 3.24e-11, 2.769e-11,
    2.361e-11, 2.011e-11, 1.71e-11, 1.453e-11, 1.233e-11, 1.045e-11,
    8.851e-12, 7.48e-12, 6.316e-12, 5.326e-12, 4.487e-12, 3.778e-12,
    3.176e-12, 2.665e-12, 2.234e-12, 1.87e-12, 1.563e-12, 1.304e-12,
    1.085e-12, 9.007e-13, 7.468e-13, 6.179e-13, 5.092e-13, 4.188e-13,
    3.442e-13, 2.816e-13, 2.304e-13, 1.885e-13, 1.542e-13, 1.263e-13,
    1.035e-13, 8.5e-14, 7.004e-14, 5.783e-14, 4.795e-14, 4.007e-14,
    3.345e-14, 2.792e-14, 2.33e-14, 1.978e-14, 1.686e-14, 1.438e-14,
    1.234e-14, 1.07e-14, 9.312e-15, 8.131e-15, 7.164e-15, 6.367e-15,
    5.67e-15, 5.088e-15, 4.565e-15, 4.138e-15, 3.769e-15, 3.432e-15,
    3.148e-15
  };

  static double clono2[121] = {
    1.011e-13, 1.515e-13, 2.272e-13, 3.446e-13, 5.231e-13, 8.085e-13,
    1.253e-12, 1.979e-12, 3.149e-12, 5.092e-12, 8.312e-12, 1.366e-11,
    2.272e-11, 3.791e-11, 6.209e-11, 9.101e-11, 1.334e-10, 1.951e-10,
    2.853e-10, 3.94e-10, 4.771e-10, 5.771e-10, 6.675e-10, 7.665e-10,
    8.504e-10, 8.924e-10, 9.363e-10, 8.923e-10, 8.411e-10, 7.646e-10,
    6.525e-10, 5.576e-10, 4.398e-10, 3.403e-10, 2.612e-10, 1.915e-10,
    1.407e-10, 1.028e-10, 7.455e-11, 5.42e-11, 3.708e-11, 2.438e-11,
    1.618e-11, 1.075e-11, 7.17e-12, 4.784e-12, 3.205e-12, 2.147e-12,
    1.44e-12, 9.654e-13, 6.469e-13, 4.332e-13, 2.891e-13, 1.926e-13,
    1.274e-13, 8.422e-14, 5.547e-14, 3.636e-14, 2.368e-14, 1.536e-14,
    9.937e-15, 6.39e-15, 4.101e-15, 2.61e-15, 1.659e-15, 1.052e-15,
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    6.638e-16, 4.172e-16, 2.61e-16, 1.63e-16, 1.013e-16, 6.275e-17,
    3.879e-17, 2.383e-17, 1.461e-17, 8.918e-18, 5.43e-18, 3.301e-18,
    1.997e-18, 1.203e-18, 7.216e-19, 4.311e-19, 2.564e-19, 1.519e-19,
    8.911e-20, 5.203e-20, 3.026e-20, 1.748e-20, 9.99e-21, 5.673e-21,
    3.215e-21, 1.799e-21, 1.006e-21, 5.628e-22, 3.146e-22, 1.766e-22,
    9.94e-23, 5.614e-23, 3.206e-23, 1.841e-23, 1.071e-23, 6.366e-24,
    3.776e-24, 2.238e-24, 1.326e-24, 8.253e-25, 5.201e-25, 3.279e-25,
    2.108e-25, 1.395e-25, 9.326e-26, 6.299e-26, 4.365e-26, 3.104e-26,
    2.219e-26, 1.621e-26, 1.185e-26, 8.92e-27, 6.804e-27, 5.191e-27,
    4.041e-27
  };

  static double co[121] = {
    1.907e-07, 1.553e-07, 1.362e-07, 1.216e-07, 1.114e-07, 1.036e-07,
    9.737e-08, 9.152e-08, 8.559e-08, 7.966e-08, 7.277e-08, 6.615e-08,
    5.884e-08, 5.22e-08, 4.699e-08, 4.284e-08, 3.776e-08, 3.274e-08,
    2.845e-08, 2.479e-08, 2.246e-08, 2.054e-08, 1.991e-08, 1.951e-08,
    1.94e-08, 2.009e-08, 2.1e-08, 2.201e-08, 2.322e-08, 2.45e-08,
    2.602e-08, 2.73e-08, 2.867e-08, 2.998e-08, 3.135e-08, 3.255e-08,
    3.352e-08, 3.426e-08, 3.484e-08, 3.53e-08, 3.593e-08, 3.671e-08,
    3.759e-08, 3.945e-08, 4.192e-08, 4.49e-08, 5.03e-08, 5.703e-08,
    6.538e-08, 7.878e-08, 9.644e-08, 1.196e-07, 1.498e-07, 1.904e-07,
    2.422e-07, 3.055e-07, 3.804e-07, 4.747e-07, 5.899e-07, 7.272e-07,
    8.91e-07, 1.071e-06, 1.296e-06, 1.546e-06, 1.823e-06, 2.135e-06,
    2.44e-06, 2.714e-06, 2.967e-06, 3.189e-06, 3.391e-06, 3.58e-06,
    3.773e-06, 4.022e-06, 4.346e-06, 4.749e-06, 5.199e-06, 5.668e-06,
    6.157e-06, 6.688e-06, 7.254e-06, 7.867e-06, 8.539e-06, 9.26e-06,
    1.009e-05, 1.119e-05, 1.228e-05, 1.365e-05, 1.506e-05, 1.641e-05,
    1.784e-05, 1.952e-05, 2.132e-05, 2.323e-05, 2.531e-05, 2.754e-05,
    3.047e-05, 3.459e-05, 3.922e-05, 4.439e-05, 4.825e-05, 5.077e-05,
    5.34e-05, 5.618e-05, 5.909e-05, 6.207e-05, 6.519e-05, 6.845e-05,
    6.819e-05, 6.726e-05, 6.622e-05, 6.512e-05, 6.671e-05, 6.862e-05,
    7.048e-05, 7.264e-05, 7.3e-05, 7.3e-05, 7.3e-05, 7.3e-05, 7.3e-05
  };

  static double cof2[121] = {
    7.5e-14, 1.055e-13, 1.485e-13, 2.111e-13, 3.001e-13, 4.333e-13,
    6.269e-13, 9.221e-13, 1.364e-12, 2.046e-12, 3.093e-12, 4.703e-12,
    7.225e-12, 1.113e-11, 1.66e-11, 2.088e-11, 2.626e-11, 3.433e-11,
    4.549e-11, 5.886e-11, 7.21e-11, 8.824e-11, 1.015e-10, 1.155e-10,
    1.288e-10, 1.388e-10, 1.497e-10, 1.554e-10, 1.606e-10, 1.639e-10,
    1.64e-10, 1.64e-10, 1.596e-10, 1.542e-10, 1.482e-10, 1.382e-10,
    1.289e-10, 1.198e-10, 1.109e-10, 1.026e-10, 9.484e-11, 8.75e-11,
    8.086e-11, 7.49e-11, 6.948e-11, 6.446e-11, 5.961e-11, 5.505e-11,
    5.085e-11, 4.586e-11, 4.1e-11, 3.665e-11, 3.235e-11, 2.842e-11,
    2.491e-11, 2.11e-11, 1.769e-11, 1.479e-11, 1.197e-11, 9.631e-12,
    7.74e-12, 6.201e-12, 4.963e-12, 3.956e-12, 3.151e-12, 2.507e-12,
    1.99e-12, 1.576e-12, 1.245e-12, 9.83e-13, 7.742e-13, 6.088e-13,
    4.782e-13, 3.745e-13, 2.929e-13, 2.286e-13, 1.782e-13, 1.388e-13,
    1.079e-13, 8.362e-14, 6.471e-14, 4.996e-14, 3.85e-14, 2.96e-14,
    2.265e-14, 1.729e-14, 1.317e-14, 9.998e-15, 7.549e-15, 5.683e-15,
    4.273e-15, 3.193e-15, 2.385e-15, 1.782e-15, 1.331e-15, 9.957e-16,
    7.461e-16, 5.601e-16, 4.228e-16, 3.201e-16, 2.438e-16, 1.878e-16,
    1.445e-16, 1.111e-16, 8.544e-17, 6.734e-17, 5.341e-17, 4.237e-17,
    3.394e-17, 2.759e-17, 2.254e-17, 1.851e-17, 1.54e-17, 1.297e-17,
    1.096e-17, 9.365e-18, 8e-18, 6.938e-18, 6.056e-18, 5.287e-18,
    4.662e-18
  };

  static double f11[121] = {
    2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10,
    2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.65e-10, 2.635e-10, 2.536e-10,
    2.44e-10, 2.348e-10, 2.258e-10, 2.153e-10, 2.046e-10, 1.929e-10,
    1.782e-10, 1.648e-10, 1.463e-10, 1.291e-10, 1.1e-10, 8.874e-11,
    7.165e-11, 5.201e-11, 3.744e-11, 2.577e-11, 1.64e-11, 1.048e-11,
    5.993e-12, 3.345e-12, 1.839e-12, 9.264e-13, 4.688e-13, 2.329e-13,
    1.129e-13, 5.505e-14, 2.825e-14, 1.492e-14, 7.997e-15, 5.384e-15,
    3.988e-15, 2.955e-15, 2.196e-15, 1.632e-15, 1.214e-15, 9.025e-16,
    6.708e-16, 4.984e-16, 3.693e-16, 2.733e-16, 2.013e-16, 1.481e-16,
    1.087e-16, 7.945e-17, 5.782e-17, 4.195e-17, 3.038e-17, 2.19e-17,
    1.577e-17, 1.128e-17, 8.063e-18, 5.753e-18, 4.09e-18, 2.899e-18,
    2.048e-18, 1.444e-18, 1.015e-18, 7.12e-19, 4.985e-19, 3.474e-19,
    2.417e-19, 1.677e-19, 1.161e-19, 8.029e-20, 5.533e-20, 3.799e-20,
    2.602e-20, 1.776e-20, 1.209e-20, 8.202e-21, 5.522e-21, 3.707e-21,
    2.48e-21, 1.652e-21, 1.091e-21, 7.174e-22, 4.709e-22, 3.063e-22,
    1.991e-22, 1.294e-22, 8.412e-23, 5.483e-23, 3.581e-23, 2.345e-23,
    1.548e-23, 1.027e-23, 6.869e-24, 4.673e-24, 3.173e-24, 2.153e-24,
    1.461e-24, 1.028e-24, 7.302e-25, 5.188e-25, 3.739e-25, 2.753e-25,
    2.043e-25, 1.528e-25, 1.164e-25, 9.041e-26, 7.051e-26, 5.587e-26,
    4.428e-26, 3.588e-26, 2.936e-26, 2.402e-26, 1.995e-26
  };

  static double f12[121] = {
    5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10,
    5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.45e-10, 5.429e-10, 5.291e-10,
    5.155e-10, 5.022e-10, 4.893e-10, 4.772e-10, 4.655e-10, 4.497e-10,
    4.249e-10, 4.015e-10, 3.632e-10, 3.261e-10, 2.858e-10, 2.408e-10,
```

```
  2.03e-10, 1.685e-10, 1.4e-10, 1.163e-10, 9.65e-11, 8.02e-11, 6.705e-11,
  5.624e-11, 4.764e-11, 4.249e-11, 3.792e-11, 3.315e-11, 2.819e-11,
  2.4e-11, 1.999e-11, 1.64e-11, 1.352e-11, 1.14e-11, 9.714e-12,
  8.28e-12, 7.176e-12, 6.251e-12, 5.446e-12, 4.72e-12, 4.081e-12,
  3.528e-12, 3.08e-12, 2.699e-12, 2.359e-12, 2.111e-12, 1.901e-12,
  1.709e-12, 1.534e-12, 1.376e-12, 1.233e-12, 1.103e-12, 9.869e-13,
  8.808e-13, 7.859e-13, 7.008e-13, 6.241e-13, 5.553e-13, 4.935e-13,
  4.383e-13, 3.889e-13, 3.447e-13, 3.054e-13, 2.702e-13, 2.389e-13,
  2.11e-13, 1.862e-13, 1.643e-13, 1.448e-13, 1.274e-13, 1.121e-13,
  9.844e-14, 8.638e-14, 7.572e-14, 6.62e-14, 5.782e-14, 5.045e-14,
  4.394e-14, 3.817e-14, 3.311e-14, 2.87e-14, 2.48e-14, 2.142e-14,
  1.851e-14, 1.599e-14, 1.383e-14, 1.196e-14, 1.036e-14, 9e-15,
  7.828e-15, 6.829e-15, 5.992e-15, 5.254e-15, 4.606e-15, 4.037e-15,
  3.583e-15, 3.19e-15, 2.841e-15, 2.542e-15, 2.291e-15, 2.07e-15,
  1.875e-15, 1.71e-15, 1.57e-15, 1.442e-15, 1.333e-15, 1.232e-15,
  1.147e-15, 1.071e-15, 1.001e-15, 9.396e-16
};

static double f14[121] = {
  9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 9e-11,
  9e-11, 9e-11, 9e-11, 9e-11, 9e-11, 8.91e-11, 8.73e-11, 8.46e-11,
  8.19e-11, 7.92e-11, 7.74e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11,
  7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11, 7.65e-11
};

static double f22[121] = {
  1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10, 1.4e-10,
  1.4e-10, 1.4e-10, 1.4e-10, 1.372e-10, 1.317e-10, 1.235e-10, 1.153e-10,
  1.075e-10, 1.002e-10, 9.332e-11, 8.738e-11, 8.194e-11, 7.7e-11,
  7.165e-11, 6.753e-11, 6.341e-11, 5.971e-11, 5.6e-11, 5.229e-11,
  4.859e-11, 4.488e-11, 4.118e-11, 3.83e-11, 3.568e-11, 3.308e-11,
  3.047e-11, 2.82e-11, 2.594e-11, 2.409e-11, 2.237e-11, 2.065e-11,
  1.894e-11, 1.771e-11, 1.647e-11, 1.532e-11, 1.416e-11, 1.332e-11,
  1.246e-11, 1.161e-11, 1.087e-11, 1.017e-11, 9.471e-12, 8.853e-12,
  8.235e-12, 7.741e-12, 7.247e-12, 6.836e-12, 6.506e-12, 6.176e-12,
  5.913e-12, 5.65e-12, 5.419e-12, 5.221e-12, 5.024e-12, 4.859e-12,
  4.694e-12, 4.546e-12, 4.414e-12, 4.282e-12, 4.15e-12, 4.019e-12,
  3.903e-12, 3.805e-12, 3.706e-12, 3.607e-12, 3.508e-12, 3.41e-12,
  3.31e-12, 3.212e-12, 3.129e-12, 3.047e-12, 2.964e-12, 2.882e-12,
  2.8e-12, 2.734e-12, 2.668e-12, 2.602e-12, 2.537e-12, 2.471e-12,
  2.421e-12, 2.372e-12, 2.322e-12, 2.273e-12, 2.224e-12, 2.182e-12,
  2.141e-12, 2.1e-12, 2.059e-12, 2.018e-12, 1.977e-12, 1.935e-12,
  1.894e-12, 1.853e-12, 1.812e-12, 1.77e-12, 1.73e-12, 1.688e-12,
  1.647e-12, 1.606e-12, 1.565e-12, 1.524e-12, 1.483e-12, 1.441e-12,
  1.4e-12, 1.359e-12, 1.317e-12, 1.276e-12, 1.235e-12, 1.194e-12,
  1.153e-12, 1.112e-12, 1.071e-12, 1.029e-12, 9.883e-13
};

static double h2o[121] = {
  0.01166, 0.008269, 0.005742, 0.003845, 0.00277, 0.001897, 0.001272,
  0.000827, 0.000539, 0.0003469, 0.0001579, 3.134e-05, 1.341e-05,
  6.764e-06, 4.498e-06, 3.703e-06, 3.724e-06, 3.899e-06, 4.002e-06,
  4.122e-06, 4.277e-06, 4.438e-06, 4.558e-06, 4.673e-06, 4.763e-06,
  4.809e-06, 4.856e-06, 4.936e-06, 5.021e-06, 5.114e-06, 5.222e-06,
  5.331e-06, 5.414e-06, 5.488e-06, 5.563e-06, 5.633e-06, 5.704e-06,
  5.767e-06, 5.819e-06, 5.872e-06, 5.914e-06, 5.949e-06, 5.984e-06,
  6.015e-06, 6.044e-06, 6.073e-06, 6.104e-06, 6.136e-06, 6.167e-06,
  6.189e-06, 6.208e-06, 6.226e-06, 6.212e-06, 6.185e-06, 6.158e-06,
  6.114e-06, 6.066e-06, 6.018e-06, 5.877e-06, 5.728e-06, 5.582e-06,
  5.437e-06, 5.296e-06, 5.156e-06, 5.02e-06, 4.886e-06, 4.754e-06,
  4.625e-06, 4.498e-06, 4.374e-06, 4.242e-06, 4.096e-06, 3.955e-06,
  3.817e-06, 3.683e-06, 3.491e-06, 3.204e-06, 2.94e-06, 2.696e-06,
  2.47e-06, 2.252e-06, 2.019e-06, 1.808e-06, 1.618e-06, 1.445e-06,
  1.285e-06, 1.105e-06, 9.489e-07, 8.121e-07, 6.938e-07, 5.924e-07,
  5.04e-07, 4.288e-07, 3.648e-07, 3.103e-07, 2.642e-07, 2.252e-07,
  1.921e-07, 1.643e-07, 1.408e-07, 1.211e-07, 1.048e-07, 9.063e-08,
  7.835e-08, 6.774e-08, 5.936e-08, 5.221e-08, 4.592e-08, 4.061e-08,
  3.62e-08, 3.236e-08, 2.902e-08, 2.62e-08, 2.383e-08, 2.171e-08,
  1.989e-08, 1.823e-08, 1.684e-08, 1.562e-08, 1.449e-08, 1.351e-08
};

static double h2o2[121] = {
  1.779e-10, 7.938e-10, 8.953e-10, 8.032e-10, 6.564e-10, 5.159e-10,
  4.003e-10, 3.026e-10, 2.222e-10, 1.58e-10, 1.044e-10, 6.605e-11,
```

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  3.413e-11, 1.453e-11, 1.062e-11, 1.009e-11, 9.597e-12, 1.175e-11,
  1.572e-11, 2.091e-11, 2.746e-11, 3.603e-11, 4.791e-11, 6.387e-11,
  8.239e-11, 1.007e-10, 1.23e-10, 1.363e-10, 1.489e-10, 1.585e-10,
  1.608e-10, 1.632e-10, 1.576e-10, 1.502e-10, 1.423e-10, 1.302e-10,
  1.192e-10, 1.085e-10, 9.795e-11, 8.854e-11, 8.057e-11, 7.36e-11,
  6.736e-11, 6.362e-11, 6.087e-11, 5.825e-11, 5.623e-11, 5.443e-11,
  5.27e-11, 5.098e-11, 4.931e-11, 4.769e-11, 4.611e-11, 4.458e-11,
  4.308e-11, 4.102e-11, 3.887e-11, 3.682e-11, 3.521e-11, 3.369e-11,
  3.224e-11, 3.082e-11, 2.946e-11, 2.814e-11, 2.687e-11, 2.566e-11,
  2.449e-11, 2.336e-11, 2.227e-11, 2.123e-11, 2.023e-11, 1.927e-11,
  1.835e-11, 1.746e-11, 1.661e-11, 1.58e-11, 1.502e-11, 1.428e-11,
  1.357e-11, 1.289e-11, 1.224e-11, 1.161e-11, 1.102e-11, 1.045e-11,
  9.895e-12, 9.369e-12, 8.866e-12, 8.386e-12, 7.922e-12, 7.479e-12,
  7.06e-12, 6.656e-12, 6.274e-12, 5.914e-12, 5.575e-12, 5.257e-12,
  4.959e-12, 4.679e-12, 4.42e-12, 4.178e-12, 3.954e-12, 3.75e-12,
  3.557e-12, 3.372e-12, 3.198e-12, 3.047e-12, 2.908e-12, 2.775e-12,
  2.653e-12, 2.544e-12, 2.442e-12, 2.346e-12, 2.26e-12, 2.183e-12,
  2.11e-12, 2.044e-12, 1.98e-12, 1.924e-12, 1.871e-12, 1.821e-12,
  1.775e-12
};

static double hcn[121] = {
  5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10,
  5.5e-10, 5.5e-10, 5.5e-10, 5.5e-10, 5.498e-10, 5.495e-10, 5.493e-10,
  5.49e-10, 5.488e-10, 4.717e-10, 3.946e-10, 3.174e-10, 2.4e-10,
  1.626e-10, 1.619e-10, 1.612e-10, 1.602e-10, 1.593e-10, 1.582e-10,
  1.572e-10, 1.56e-10, 1.549e-10, 1.539e-10, 1.53e-10, 1.519e-10,
  1.506e-10, 1.487e-10, 1.467e-10, 1.449e-10, 1.43e-10, 1.413e-10,
  1.397e-10, 1.382e-10, 1.368e-10, 1.354e-10, 1.337e-10, 1.315e-10,
  1.292e-10, 1.267e-10, 1.241e-10, 1.215e-10, 1.19e-10, 1.165e-10,
  1.141e-10, 1.118e-10, 1.096e-10, 1.072e-10, 1.047e-10, 1.021e-10,
  9.968e-11, 9.739e-11, 9.539e-11, 9.339e-11, 9.135e-11, 8.898e-11,
  8.664e-11, 8.439e-11, 8.249e-11, 8.075e-11, 7.904e-11, 7.735e-11,
  7.565e-11, 7.399e-11, 7.245e-11, 7.109e-11, 6.982e-11, 6.863e-11,
  6.755e-11, 6.657e-11, 6.587e-11, 6.527e-11, 6.476e-11, 6.428e-11,
  6.382e-11, 6.343e-11, 6.307e-11, 6.272e-11, 6.238e-11, 6.205e-11,
  6.17e-11, 6.137e-11, 6.102e-11, 6.072e-11, 6.046e-11, 6.03e-11,
  6.018e-11, 6.01e-11, 6.001e-11, 5.992e-11, 5.984e-11, 5.975e-11,
  5.967e-11, 5.958e-11, 5.95e-11, 5.941e-11, 5.933e-11, 5.925e-11,
  5.916e-11, 5.908e-11, 5.899e-11, 5.891e-11, 5.883e-11, 5.874e-11,
  5.866e-11, 5.858e-11, 5.85e-11, 5.841e-11, 5.833e-11, 5.825e-11,
  5.817e-11, 5.808e-11, 5.8e-11, 5.792e-11, 5.784e-11
};

static double hno3[121] = {
  1.809e-10, 7.234e-10, 5.899e-10, 4.342e-10, 3.277e-10, 2.661e-10,
  2.35e-10, 2.267e-10, 2.389e-10, 2.651e-10, 3.255e-10, 4.099e-10,
  5.42e-10, 6.978e-10, 8.807e-10, 1.112e-09, 1.405e-09, 2.04e-09,
  3.111e-09, 4.5e-09, 5.762e-09, 7.37e-09, 7.852e-09, 8.109e-09,
  8.067e-09, 7.554e-09, 7.076e-09, 6.268e-09, 5.524e-09, 4.749e-09,
  3.909e-09, 3.223e-09, 2.517e-09, 1.942e-09, 1.493e-09, 1.122e-09,
  8.449e-10, 6.361e-10, 4.787e-10, 3.611e-10, 2.804e-10, 2.215e-10,
  1.758e-10, 1.441e-10, 1.197e-10, 9.953e-11, 8.505e-11, 7.334e-11,
  6.325e-11, 5.625e-11, 5.058e-11, 4.548e-11, 4.122e-11, 3.748e-11,
  3.402e-11, 3.088e-11, 2.8e-11, 2.536e-11, 2.293e-11, 2.072e-11,
  1.871e-11, 1.687e-11, 1.52e-11, 1.368e-11, 1.23e-11, 1.105e-11,
  9.922e-12, 8.898e-12, 7.972e-12, 7.139e-12, 6.385e-12, 5.708e-12,
  5.099e-12, 4.549e-12, 4.056e-12, 3.613e-12, 3.216e-12, 2.862e-12,
  2.544e-12, 2.259e-12, 2.004e-12, 1.776e-12, 1.572e-12, 1.391e-12,
  1.227e-12, 1.082e-12, 9.528e-13, 8.379e-13, 7.349e-13, 6.436e-13,
  5.634e-13, 4.917e-13, 4.291e-13, 3.745e-13, 3.267e-13, 2.854e-13,
  2.494e-13, 2.181e-13, 1.913e-13, 1.68e-13, 1.479e-13, 1.31e-13,
  1.159e-13, 1.025e-13, 9.067e-14, 8.113e-14, 7.281e-14, 6.535e-14,
  5.892e-14, 5.348e-14, 4.867e-14, 4.439e-14, 4.073e-14, 3.76e-14,
  3.476e-14, 3.229e-14, 3e-14, 2.807e-14, 2.635e-14, 2.473e-14,
  2.332e-14
};

static double hno4[121] = {
  6.118e-12, 3.594e-12, 2.807e-12, 3.04e-12, 4.458e-12, 7.986e-12,
  1.509e-11, 2.661e-11, 3.738e-11, 4.652e-11, 4.429e-11, 3.992e-11,
  3.347e-11, 3.005e-11, 3.173e-11, 4.055e-11, 5.812e-11, 8.489e-11,
  1.19e-10, 1.482e-10, 1.766e-10, 2.103e-10, 2.35e-10, 2.598e-10,
  2.801e-10, 2.899e-10, 3e-10, 2.817e-10, 2.617e-10, 2.332e-10,
  1.933e-10, 1.605e-10, 1.232e-10, 9.285e-11, 6.941e-11, 4.951e-11,
  3.539e-11, 2.402e-11, 1.522e-11, 9.676e-12, 6.056e-12, 3.745e-12,
  2.34e-12, 1.463e-12, 9.186e-13, 5.769e-13, 3.322e-13, 1.853e-13,
  1.035e-13, 7.173e-14, 5.382e-14, 4.036e-14, 3.401e-14, 2.997e-14,
  2.635e-14, 2.316e-14, 2.034e-14, 1.783e-14, 1.56e-14, 1.363e-14,
  1.19e-14, 1.037e-14, 9.032e-15, 7.846e-15, 6.813e-15, 5.912e-15,
  5.121e-15, 4.431e-15, 3.829e-15, 3.306e-15, 2.851e-15, 2.456e-15,
  2.114e-15, 1.816e-15, 1.559e-15, 1.337e-15, 1.146e-15, 9.811e-16,
  8.389e-16, 7.162e-16, 6.109e-16, 5.203e-16, 4.425e-16, 3.76e-16,
  3.184e-16, 2.692e-16, 2.274e-16, 1.917e-16, 1.61e-16, 1.35e-16,
  1.131e-16, 9.437e-17, 7.874e-17, 6.57e-17, 5.481e-17, 4.579e-17,
  3.828e-17, 3.204e-17, 2.691e-17, 2.264e-17, 1.912e-17, 1.626e-17,
  1.382e-17, 1.174e-17, 9.972e-18, 8.603e-18, 7.45e-18, 6.453e-18,
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  5.623e-18, 4.944e-18, 4.361e-18, 3.859e-18, 3.443e-18, 3.096e-18,
  2.788e-18, 2.528e-18, 2.293e-18, 2.099e-18, 1.929e-18, 1.773e-18,
  1.64e-18
};

static double hocl[121] = {
  1.056e-12, 1.194e-12, 1.35e-12, 1.531e-12, 1.737e-12, 1.982e-12,
  2.263e-12, 2.599e-12, 2.991e-12, 3.459e-12, 4.012e-12, 4.662e-12,
  5.438e-12, 6.35e-12, 7.425e-12, 8.686e-12, 1.016e-11, 1.188e-11,
  1.389e-11, 1.659e-11, 2.087e-11, 2.621e-11, 3.265e-11, 4.064e-11,
  4.859e-11, 5.441e-11, 6.09e-11, 6.373e-11, 6.611e-11, 6.94e-11,
  7.44e-11, 7.97e-11, 8.775e-11, 9.722e-11, 1.064e-10, 1.089e-10,
  1.114e-10, 1.106e-10, 1.053e-10, 1.004e-10, 9.006e-11, 7.778e-11,
  6.739e-11, 5.636e-11, 4.655e-11, 3.845e-11, 3.042e-11, 2.368e-11,
  1.845e-11, 1.442e-11, 1.127e-11, 8.814e-12, 6.544e-12, 4.763e-12,
  3.449e-12, 2.612e-12, 1.999e-12, 1.526e-12, 1.16e-12, 8.793e-13,
  6.655e-13, 5.017e-13, 3.778e-13, 2.829e-13, 2.117e-13, 1.582e-13,
  1.178e-13, 8.755e-14, 6.486e-14, 4.799e-14, 3.54e-14, 2.606e-14,
  1.916e-14, 1.403e-14, 1.026e-14, 7.48e-15, 5.446e-15, 3.961e-15,
  2.872e-15, 2.076e-15, 1.498e-15, 1.077e-15, 7.726e-16, 5.528e-16,
  3.929e-16, 2.785e-16, 1.969e-16, 1.386e-16, 9.69e-17, 6.747e-17,
  4.692e-17, 3.236e-17, 2.232e-17, 1.539e-17, 1.061e-17, 7.332e-18,
  5.076e-18, 3.522e-18, 2.461e-18, 1.726e-18, 1.22e-18, 8.75e-19,
  6.264e-19, 4.482e-19, 3.207e-19, 2.368e-19, 1.762e-19, 1.312e-19,
  9.891e-20, 7.595e-20, 5.87e-20, 4.567e-20, 3.612e-20, 2.904e-20,
  2.343e-20, 1.917e-20, 1.568e-20, 1.308e-20, 1.1e-20, 9.25e-21,
  7.881e-21
};

static double n2o[121] = {
  3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07, 3.17e-07,
  3.17e-07, 3.17e-07, 3.17e-07, 3.124e-07, 3.077e-07, 3.03e-07,
  2.984e-07, 2.938e-07, 2.892e-07, 2.847e-07, 2.779e-07, 2.705e-07,
  2.631e-07, 2.557e-07, 2.484e-07, 2.345e-07, 2.201e-07, 2.01e-07,
  1.754e-07, 1.532e-07, 1.329e-07, 1.154e-07, 1.003e-07, 8.735e-08,
  7.617e-08, 6.512e-08, 5.547e-08, 4.709e-08, 3.915e-08, 3.259e-08,
  2.738e-08, 2.327e-08, 1.98e-08, 1.711e-08, 1.493e-08, 1.306e-08,
  1.165e-08, 1.049e-08, 9.439e-09, 8.375e-09, 7.391e-09, 6.525e-09,
  5.759e-09, 5.083e-09, 4.485e-09, 3.953e-09, 3.601e-09, 3.27e-09,
  2.975e-09, 2.757e-09, 2.556e-09, 2.37e-09, 2.195e-09, 2.032e-09,
  1.912e-09, 1.79e-09, 1.679e-09, 1.572e-09, 1.482e-09, 1.402e-09,
  1.326e-09, 1.254e-09, 1.187e-09, 1.127e-09, 1.071e-09, 1.02e-09,
  9.673e-10, 9.193e-10, 8.752e-10, 8.379e-10, 8.017e-10, 7.66e-10,
  7.319e-10, 7.004e-10, 6.721e-10, 6.459e-10, 6.199e-10, 5.942e-10,
  5.703e-10, 5.488e-10, 5.283e-10, 5.082e-10, 4.877e-10, 4.696e-10,
  4.52e-10, 4.355e-10, 4.198e-10, 4.039e-10, 3.888e-10, 3.754e-10,
  3.624e-10, 3.499e-10, 3.381e-10, 3.267e-10, 3.163e-10, 3.058e-10,
  2.959e-10, 2.864e-10, 2.77e-10, 2.686e-10, 2.604e-10, 2.534e-10,
  2.462e-10, 2.386e-10, 2.318e-10, 2.247e-10, 2.189e-10, 2.133e-10,
  2.071e-10, 2.014e-10, 1.955e-10, 1.908e-10, 1.86e-10, 1.817e-10
};

static double n2o5[121] = {
  1.231e-11, 3.035e-12, 1.702e-12, 9.877e-13, 8.081e-13, 9.039e-13,
  1.169e-12, 1.474e-12, 1.651e-12, 1.795e-12, 1.998e-12, 2.543e-12,
  4.398e-12, 7.698e-12, 1.28e-11, 2.131e-11, 3.548e-11, 5.894e-11,
  7.645e-11, 1.089e-10, 1.391e-10, 1.886e-10, 2.386e-10, 2.986e-10,
  3.487e-10, 3.994e-10, 4.5e-10, 4.6e-10, 4.591e-10, 4.1e-10, 3.488e-10,
  2.846e-10, 2.287e-10, 1.696e-10, 1.011e-10, 6.428e-11, 4.324e-11,
  2.225e-11, 6.214e-12, 3.608e-12, 8.793e-13, 4.491e-13, 1.04e-13,
  6.1e-14, 3.436e-14, 6.671e-15, 1.171e-15, 5.848e-16, 1.212e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16, 1e-16,
  1e-16, 1e-16
};

static double nh3[121] = {
  1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10,
  1e-10, 1e-10, 1e-10, 1e-10, 9.444e-11, 8.488e-11, 7.241e-11, 5.785e-11,
  4.178e-11, 3.018e-11, 2.18e-11, 1.574e-11, 1.137e-11, 8.211e-12,
  5.973e-12, 4.327e-12, 3.118e-12, 2.234e-12, 1.573e-12, 1.04e-12,
  6.762e-13, 4.202e-13, 2.406e-13, 1.335e-13, 6.938e-14, 3.105e-14,
  1.609e-14, 1.033e-14, 6.432e-15, 4.031e-15, 2.555e-15, 1.656e-15,
  1.115e-15, 7.904e-16, 5.63e-16, 4.048e-16, 2.876e-16, 2.004e-16,
  1.356e-16, 9.237e-17, 6.235e-17, 4.223e-17, 3.009e-17, 2.328e-17,
  2.002e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
```

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  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17, 1.914e-17,
  1.914e-17
};

static double no[121] = {
  2.586e-10, 4.143e-11, 1.566e-11, 9.591e-12, 8.088e-12, 8.462e-12,
  1.013e-11, 1.328e-11, 1.855e-11, 2.678e-11, 3.926e-11, 5.464e-11,
  7.012e-11, 8.912e-11, 1.127e-10, 1.347e-10, 1.498e-10, 1.544e-10,
  1.602e-10, 1.824e-10, 2.078e-10, 2.366e-10, 2.691e-10, 5.141e-10,
  8.259e-10, 1.254e-09, 1.849e-09, 2.473e-09, 3.294e-09, 4.16e-09,
  5.095e-09, 6.11e-09, 6.93e-09, 7.888e-09, 8.903e-09, 9.713e-09,
  1.052e-08, 1.115e-08, 1.173e-08, 1.21e-08, 1.228e-08, 1.239e-08,
  1.231e-08, 1.213e-08, 1.192e-08, 1.138e-08, 1.085e-08, 1.008e-08,
  9.224e-09, 8.389e-09, 7.262e-09, 6.278e-09, 5.335e-09, 4.388e-09,
  3.589e-09, 2.761e-09, 2.129e-09, 1.633e-09, 1.243e-09, 9.681e-10,
  8.355e-10, 7.665e-10, 7.442e-10, 8.584e-10, 9.732e-10, 1.063e-09,
  1.163e-09, 1.286e-09, 1.472e-09, 1.707e-09, 2.032e-09, 2.474e-09,
  2.977e-09, 3.506e-09, 4.102e-09, 5.013e-09, 6.493e-09, 8.414e-09,
  1.077e-08, 1.367e-08, 1.777e-08, 2.625e-08, 3.926e-08, 5.545e-08,
  7.195e-08, 9.464e-08, 1.404e-07, 2.183e-07, 3.329e-07, 4.535e-07,
  6.158e-07, 8.187e-07, 1.075e-06, 1.422e-06, 1.979e-06, 2.71e-06,
  3.58e-06, 4.573e-06, 5.951e-06, 7.999e-06, 1.072e-05, 1.372e-05,
  1.697e-05, 2.112e-05, 2.643e-05, 3.288e-05, 3.994e-05, 4.794e-05,
  5.606e-05, 6.383e-05, 7.286e-05, 8.156e-05, 8.883e-05, 9.469e-05,
  9.848e-05, 0.0001023, 0.0001066, 0.0001115, 0.0001145, 0.0001142,
  0.0001133
};

static double no2[121] = {
  3.036e-09, 2.945e-10, 9.982e-11, 5.069e-11, 3.485e-11, 2.982e-11,
  2.947e-11, 3.164e-11, 3.714e-11, 4.586e-11, 6.164e-11, 8.041e-11,
  9.982e-11, 1.283e-10, 1.73e-10, 2.56e-10, 3.909e-10, 5.959e-10,
  9.081e-10, 1.384e-09, 1.788e-09, 2.189e-09, 2.686e-09, 3.091e-09,
  3.49e-09, 3.796e-09, 4.2e-09, 5.103e-09, 6.005e-09, 6.3e-09, 6.706e-09,
  7.07e-09, 7.434e-09, 7.663e-09, 7.788e-09, 7.8e-09, 7.597e-09,
  7.482e-09, 7.227e-09, 6.403e-09, 5.585e-09, 4.606e-09, 3.703e-09,
  2.984e-09, 2.183e-09, 1.48e-09, 8.441e-10, 5.994e-10, 3.799e-10,
  2.751e-10, 1.927e-10, 1.507e-10, 1.102e-10, 6.971e-11, 5.839e-11,
  3.904e-11, 3.087e-11, 2.176e-11, 1.464e-11, 1.209e-11, 8.497e-12,
  6.477e-12, 4.371e-12, 2.914e-12, 2.424e-12, 1.753e-12, 1.35e-12,
  9.417e-13, 6.622e-13, 5.148e-13, 3.841e-13, 3.446e-13, 3.01e-13,
  2.551e-13, 2.151e-13, 1.829e-13, 1.64e-13, 1.475e-13, 1.352e-13,
  1.155e-13, 9.963e-14, 9.771e-14, 9.577e-14, 9.384e-14, 9.186e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14,
  9e-14, 9e-14, 9e-14, 9e-14, 9e-14, 9e-14
};

static double o3[121] = {
  2.218e-08, 3.394e-08, 3.869e-08, 4.219e-08, 4.501e-08, 4.778e-08,
  5.067e-08, 5.402e-08, 5.872e-08, 6.521e-08, 7.709e-08, 9.461e-08,
  1.269e-07, 1.853e-07, 2.723e-07, 3.964e-07, 5.773e-07, 8.2e-07,
  1.155e-06, 1.59e-06, 2.076e-06, 2.706e-06, 3.249e-06, 3.848e-06,
  4.459e-06, 4.986e-06, 5.573e-06, 5.958e-06, 6.328e-06, 6.661e-06,
  6.9e-06, 7.146e-06, 7.276e-06, 7.374e-06, 7.447e-06, 7.383e-06,
  7.321e-06, 7.161e-06, 6.879e-06, 6.611e-06, 6.216e-06, 5.765e-06,
  5.355e-06, 4.905e-06, 4.471e-06, 4.075e-06, 3.728e-06, 3.413e-06,
  3.125e-06, 2.856e-06, 2.607e-06, 2.379e-06, 2.17e-06, 1.978e-06,
  1.8e-06, 1.646e-06, 1.506e-06, 1.376e-06, 1.233e-06, 1.102e-06,
  9.839e-07, 8.771e-07, 7.814e-07, 6.947e-07, 6.102e-07, 5.228e-07,
  4.509e-07, 3.922e-07, 3.501e-07, 3.183e-07, 2.909e-07, 2.686e-07,
  2.476e-07, 2.284e-07, 2.109e-07, 2.003e-07, 2.013e-07, 2.022e-07,
  2.032e-07, 2.042e-07, 2.097e-07, 2.361e-07, 2.656e-07, 2.989e-07,
  3.37e-07, 3.826e-07, 4.489e-07, 5.26e-07, 6.189e-07, 7.312e-07,
  8.496e-07, 8.444e-07, 8.392e-07, 8.339e-07, 8.286e-07, 8.234e-07,
  8.181e-07, 8.129e-07, 8.077e-07, 8.026e-07, 6.918e-07, 5.176e-07,
  3.865e-07, 2.885e-07, 2.156e-07, 1.619e-07, 1.219e-07, 9.161e-08,
  6.972e-08, 5.399e-08, 3.498e-08, 2.111e-08, 1.322e-08, 8.482e-09,
  5.527e-09, 3.423e-09, 2.071e-09, 1.314e-09, 8.529e-10, 5.503e-10,
  3.665e-10
};

static double ocs[121] = {
  6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 6e-10, 5.997e-10,
  5.989e-10, 5.881e-10, 5.765e-10, 5.433e-10, 5.074e-10, 4.567e-10,
  4.067e-10, 3.601e-10, 3.093e-10, 2.619e-10, 2.232e-10, 1.805e-10,
  1.46e-10, 1.187e-10, 8.03e-11, 5.435e-11, 3.686e-11, 2.217e-11,
  1.341e-11, 8.756e-12, 4.511e-12, 2.37e-12, 1.264e-12, 8.28e-13,
  5.263e-13, 3.209e-13, 1.717e-13, 9.068e-14, 4.709e-14, 2.389e-14,
  1.236e-14, 1.127e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
```

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  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14, 1.091e-14,
  1.091e-14, 1.091e-14, 1.091e-14
};

static double sf6[121] = {
  4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12, 4.103e-12,
  4.103e-12, 4.103e-12, 4.103e-12, 4.087e-12, 4.064e-12, 4.023e-12,
  3.988e-12, 3.941e-12, 3.884e-12, 3.755e-12, 3.622e-12, 3.484e-12,
  3.32e-12, 3.144e-12, 2.978e-12, 2.811e-12, 2.653e-12, 2.489e-12,
  2.332e-12, 2.199e-12, 2.089e-12, 2.013e-12, 1.953e-12, 1.898e-12,
  1.859e-12, 1.826e-12, 1.798e-12, 1.776e-12, 1.757e-12, 1.742e-12,
  1.728e-12, 1.717e-12, 1.707e-12, 1.698e-12, 1.691e-12, 1.685e-12,
  1.679e-12, 1.675e-12, 1.671e-12, 1.668e-12, 1.665e-12, 1.663e-12,
  1.661e-12, 1.659e-12, 1.658e-12, 1.657e-12, 1.656e-12, 1.655e-12,
  1.654e-12, 1.653e-12, 1.653e-12, 1.652e-12, 1.652e-12, 1.652e-12,
  1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12, 1.651e-12,
  1.651e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12,
  1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12, 1.65e-12
};

static double so2[121] = {
  1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10, 1e-10,
  1e-10, 1e-10, 9.867e-11, 9.537e-11, 9e-11, 8.404e-11, 7.799e-11,
  7.205e-11, 6.616e-11, 6.036e-11, 5.475e-11, 5.007e-11, 4.638e-11,
  4.346e-11, 4.055e-11, 3.763e-11, 3.471e-11, 3.186e-11, 2.905e-11,
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  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10,
  2e-10, 2e-10, 2e-10, 2e-10, 2e-10, 2e-10
};

static int ig_co2 = -999;

double *q[NG] = { NULL };

/* Find emitter index of CO2... */
if (ig_co2 == -999)
  ig_co2 = find_emitter(ctl, "CO2");

/* Identify variable... */
for (int ig = 0; ig < ctl->ng; ig++) {
  q[ig] = NULL;
  if (strcasecmp(ctl->emitter[ig], "C2H2") == 0)
    q[ig] = c2h2;
  if (strcasecmp(ctl->emitter[ig], "C2H6") == 0)
    q[ig] = c2h6;
  if (strcasecmp(ctl->emitter[ig], "CCl4") == 0)
    q[ig] = ccl4;
  if (strcasecmp(ctl->emitter[ig], "CH4") == 0)
    q[ig] = ch4;
  if (strcasecmp(ctl->emitter[ig], "ClO") == 0)
    q[ig] = clo;
  if (strcasecmp(ctl->emitter[ig], "ClONO2") == 0)
    q[ig] = clono2;
  if (strcasecmp(ctl->emitter[ig], "CO") == 0)
    q[ig] = co;
  if (strcasecmp(ctl->emitter[ig], "COF2") == 0)
    q[ig] = cof2;
  if (strcasecmp(ctl->emitter[ig], "F11") == 0)
    q[ig] = f11;
  if (strcasecmp(ctl->emitter[ig], "F12") == 0)
    q[ig] = f12;
  if (strcasecmp(ctl->emitter[ig], "F14") == 0)
    q[ig] = f14;
  if (strcasecmp(ctl->emitter[ig], "F22") == 0)
    q[ig] = f22;
```

```
    if (strcasecmp(ctl->emitter[ig], "H2O") == 0)
      q[ig] = h2o;
    if (strcasecmp(ctl->emitter[ig], "H2O2") == 0)
      q[ig] = h2o2;
    if (strcasecmp(ctl->emitter[ig], "HCN") == 0)
      q[ig] = hcn;
    if (strcasecmp(ctl->emitter[ig], "HNO3") == 0)
      q[ig] = hno3;
    if (strcasecmp(ctl->emitter[ig], "HNO4") == 0)
      q[ig] = hno4;
    if (strcasecmp(ctl->emitter[ig], "HOCl") == 0)
      q[ig] = hocl;
    if (strcasecmp(ctl->emitter[ig], "N2O") == 0)
      q[ig] = n2o;
    if (strcasecmp(ctl->emitter[ig], "N2O5") == 0)
      q[ig] = n2o5;
    if (strcasecmp(ctl->emitter[ig], "NH3") == 0)
      q[ig] = nh3;
    if (strcasecmp(ctl->emitter[ig], "NO") == 0)
      q[ig] = no;
    if (strcasecmp(ctl->emitter[ig], "NO2") == 0)
      q[ig] = no2;
    if (strcasecmp(ctl->emitter[ig], "O3") == 0)
      q[ig] = o3;
    if (strcasecmp(ctl->emitter[ig], "OCS") == 0)
      q[ig] = ocs;
    if (strcasecmp(ctl->emitter[ig], "SF6") == 0)
      q[ig] = sf6;
    if (strcasecmp(ctl->emitter[ig], "SO2") == 0)
      q[ig] = so2;
  }

  /* Loop over atmospheric data points... */
  for (int ip = 0; ip < atm->np; ip++) {

    /* Get altitude index... */
    int iz = locate_reg(z, 121, atm->z[ip]);

    /* Interpolate pressure... */
    atm->p[ip] = EXP(z[iz], pre[iz], z[iz + 1], pre[iz + 1], atm->z[ip]);

    /* Interpolate temperature... */
    atm->t[ip] = LIN(z[iz], tem[iz], z[iz + 1], tem[iz + 1], atm->z[ip]);

    /* Interpolate trace gases... */
    for (int ig = 0; ig < ctl->ng; ig++)
      if (q[ig] != NULL)
        atm->q[ig][ip] =
          LIN(z[iz], q[ig][iz], z[iz + 1], q[ig][iz + 1], atm->z[ip]);
      else
        atm->q[ig][ip] = 0;

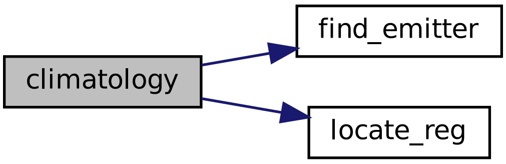
    /* Set CO2... */
    if (ig_co2 >= 0)
      atm->q[ig_co2][ip] =
        371.789948e-6 + 2.026214e-6 * (atm->time[ip] - 63158400.) / 31557600.;

    /* Set extinction to zero... */
    for (int iw = 0; iw < ctl->nw; iw++)
      atm->k[iw][ip] = 0;

    /* Set cloud layer... */
    atm->clz = atm->cldz = 0;
    for (int icl = 0; icl < ctl->ncl; icl++)
      atm->clk[icl] = 0;

    /* Set surface layer... */
    atm->sfz = atm->sfp = atm->sft = 0;
    for (int isf = 0; isf < ctl->nsf; isf++)
      atm->sfeps[isf] = 1;
  }
}
```

Here is the call graph for this function:



5.19.3.6 ctmco2()

```
double ctmco2 (
        double nu,
        double p,
        double t,
        double u )
```

Compute carbon dioxide continuum (optical depth).

Definition at line 897 of file jurassic.c.

```
         {

static double co2296[2001] = { 9.3388e-5, 9.7711e-5, 1.0224e-4, 1.0697e-4,
  1.1193e-4, 1.1712e-4, 1.2255e-4, 1.2824e-4, 1.3419e-4, 1.4043e-4,
  1.4695e-4, 1.5378e-4, 1.6094e-4, 1.6842e-4, 1.7626e-4, 1.8447e-4,
  1.9307e-4, 2.0207e-4, 2.1149e-4, 2.2136e-4, 2.3169e-4, 2.4251e-4,
  2.5384e-4, 2.657e-4, 2.7813e-4, 2.9114e-4, 3.0477e-4, 3.1904e-4,
  3.3399e-4, 3.4965e-4, 3.6604e-4, 3.8322e-4, 4.0121e-4, 4.2006e-4,
  4.398e-4, 4.6047e-4, 4.8214e-4, 5.0483e-4, 5.286e-4, 5.535e-4,
  5.7959e-4, 6.0693e-4, 6.3557e-4, 6.6558e-4, 6.9702e-4, 7.2996e-4,
  7.6449e-4, 8.0066e-4, 8.3856e-4, 8.7829e-4, 9.1991e-4, 9.6354e-4,
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    1.4731, 1.3794, 1.2921, 1.2107, 1.1346, 1.0637, .99744, .93554,
    .87771, .82368, .77313, .72587, .6816, .64014, .60134, .565,
    .53086, .49883, .46881, .44074, .4144, .38979, .36679, .34513,
```

```
    .32474, .30552, .28751, .27045, .25458, .23976, .22584, .21278,
    .20051, .18899, .17815, .16801, .15846, .14954, .14117, .13328,
    .12584
  };

  /* Get CO2 continuum absorption... */
  double xw = nu / 2 + 1;
  if (xw >= 1 && xw < 2001) {
    int iw = (int) xw;
    double dw = xw - iw;
    double ew = 1 - dw;
    double cw296 = ew * co2296[iw - 1] + dw * co2296[iw];
    double cw260 = ew * co2260[iw - 1] + dw * co2260[iw];
    double cw230 = ew * co2230[iw - 1] + dw * co2230[iw];
    double dt230 = t - 230;
    double dt260 = t - 260;
    double dt296 = t - 296;
    double ctw = dt260 * 5.050505e-4 * dt296 * cw230 - dt230 * 9.259259e-4
      * dt296 * cw260 + dt230 * 4.208754e-4 * dt260 * cw296;
    return u / NA / 1000 * p / P0 * ctw;
  } else
    return 0;
}
```

5.19.3.7 ctmh2o()

```
double ctmh2o (
        double nu,
        double p,
        double t,
        double q,
        double u )
```

Compute water vapor continuum (optical depth).

Definition at line 1755 of file jurassic.c.

```
                {

  static double h2o296[2001] = { .17, .1695, .172, .168, .1687, .1624, .1606,
    .1508, .1447, .1344, .1214, .1133, .1009, .09217, .08297, .06989,
    .06513, .05469, .05056, .04417, .03779, .03484, .02994, .0272,
    .02325, .02063, .01818, .01592, .01405, .01251, .0108, .009647,
    .008424, .007519, .006555, .00588, .005136, .004511, .003989,
    .003509, .003114, .00274, .002446, .002144, .001895, .001676,
    .001486, .001312, .001164, .001031, 9.129e-4, 8.106e-4, 7.213e-4,
    6.4e-4, 5.687e-4, 5.063e-4, 4.511e-4, 4.029e-4, 3.596e-4,
    3.22e-4, 2.889e-4, 2.597e-4, 2.337e-4, 2.108e-4, 1.907e-4,
    1.728e-4, 1.57e-4, 1.43e-4, 1.305e-4, 1.195e-4, 1.097e-4,
    1.009e-4, 9.307e-5, 8.604e-5, 7.971e-5, 7.407e-5, 6.896e-5,
    6.433e-5, 6.013e-5, 5.631e-5, 5.283e-5, 4.963e-5, 4.669e-5,
    4.398e-5, 4.148e-5, 3.917e-5, 3.702e-5, 3.502e-5, 3.316e-5,
    3.142e-5, 2.978e-5, 2.825e-5, 2.681e-5, 2.546e-5, 2.419e-5,
    2.299e-5, 2.186e-5, 2.079e-5, 1.979e-5, 1.884e-5, 1.795e-5,
    1.711e-5, 1.633e-5, 1.559e-5, 1.49e-5, 1.426e-5, 1.367e-5,
    1.312e-5, 1.263e-5, 1.218e-5, 1.178e-5, 1.143e-5, 1.112e-5,
    1.088e-5, 1.07e-5, 1.057e-5, 1.05e-5, 1.051e-5, 1.059e-5,
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```

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4.353e-11, 4.963e-11, 5.478e-11, 5.903e-11, 6.233e-11, 6.483e-11,
6.904e-11, 7.569e-11, 8.719e-11, 1.048e-10, 1.278e-10, 1.557e-10,
1.869e-10, 2.218e-10, 2.61e-10, 2.975e-10, 3.371e-10, 3.746e-10,
4.065e-10, 4.336e-10, 4.503e-10, 4.701e-10, 4.8e-10, 4.917e-10,
5.038e-10, 5.128e-10, 5.143e-10, 5.071e-10, 5.019e-10, 5.025e-10,
5.183e-10, 5.496e-10, 5.877e-10, 6.235e-10, 6.42e-10, 6.234e-10,
5.698e-10, 4.916e-10, 4.022e-10, 3.126e-10, 2.282e-10, 1.639e-10,
1.142e-10, 7.919e-11, 5.69e-11, 4.313e-11, 3.413e-11, 2.807e-11,
2.41e-11, 2.166e-11, 2.024e-11, 1.946e-11, 1.929e-11, 1.963e-11,
2.035e-11, 2.162e-11, 2.305e-11, 2.493e-11, 2.748e-11, 3.048e-11,
3.413e-11, 3.754e-11, 4.155e-11, 4.635e-11, 5.11e-11, 5.734e-11,
6.338e-11, 6.99e-11, 7.611e-11, 8.125e-11, 8.654e-11, 8.951e-11,
9.182e-11, 9.31e-11, 9.273e-11, 9.094e-11, 8.849e-11, 8.662e-11,
8.67e-11, 8.972e-11, 9.566e-11, 1.025e-10, 1.083e-10, 1.111e-10,
1.074e-10, 9.771e-11, 8.468e-11, 6.958e-11, 5.47e-11, 4.04e-11,
2.94e-11, 2.075e-11, 1.442e-11, 1.01e-11, 7.281e-12, 5.409e-12,
4.138e-12, 3.304e-12, 2.784e-12, 2.473e-12, 2.273e-12, 2.186e-12,
2.118e-12, 2.066e-12, 1.958e-12, 1.818e-12, 1.675e-12, 1.509e-12,
```

```
1.349e-12, 1.171e-12, 9.838e-13, 8.213e-13, 6.765e-13, 5.378e-13,
4.161e-13, 3.119e-13, 2.279e-13, 1.637e-13, 1.152e-13, 8.112e-14,
5.919e-14, 4.47e-14, 3.492e-14, 2.811e-14, 2.319e-14, 1.948e-14,
1.66e-14, 1.432e-14, 1.251e-14, 1.109e-14, 1.006e-14, 9.45e-15,
9.384e-15, 1.012e-14, 1.216e-14, 1.636e-14, 2.305e-14, 3.488e-14,
5.572e-14, 8.479e-14, 1.265e-13, 1.905e-13, 2.73e-13, 3.809e-13,
4.955e-13, 6.303e-13, 7.861e-13, 9.427e-13, 1.097e-12, 1.212e-12,
1.328e-12, 1.415e-12, 1.463e-12, 1.495e-12, 1.571e-12, 1.731e-12,
1.981e-12, 2.387e-12, 2.93e-12, 3.642e-12, 4.584e-12, 5.822e-12,
7.278e-12, 9.193e-12, 1.135e-11, 1.382e-11, 1.662e-11, 1.958e-11,
2.286e-11, 2.559e-11, 2.805e-11, 2.988e-11, 3.106e-11, 3.182e-11,
3.2e-11, 3.258e-11, 3.362e-11, 3.558e-11, 3.688e-11, 3.8e-11,
3.929e-11, 4.062e-11, 4.186e-11, 4.293e-11, 4.48e-11, 4.643e-11,
4.704e-11, 4.571e-11, 4.206e-11, 3.715e-11, 3.131e-11, 2.541e-11,
1.978e-11, 1.508e-11, 1.146e-11, 8.7e-12, 6.603e-12, 5.162e-12,
4.157e-12, 3.408e-12, 2.829e-12, 2.405e-12, 2.071e-12, 1.826e-12,
1.648e-12, 1.542e-12, 1.489e-12, 1.485e-12, 1.493e-12, 1.545e-12,
1.637e-12, 1.814e-12, 2.061e-12, 2.312e-12, 2.651e-12, 3.03e-12,
3.46e-12, 3.901e-12, 4.306e-12, 4.721e-12, 5.008e-12, 5.281e-12,
5.541e-12, 5.791e-12, 6.115e-12, 6.442e-12, 6.68e-12, 6.791e-12,
6.831e-12, 6.839e-12, 6.946e-12, 7.128e-12, 7.537e-12, 8.036e-12,
8.392e-12, 8.526e-12, 8.11e-12, 7.325e-12, 6.329e-12, 5.183e-12,
4.081e-12, 2.985e-12, 2.141e-12, 1.492e-12, 1.015e-12, 6.684e-13,
4.414e-13, 2.987e-13, 2.038e-13, 1.391e-13, 9.86e-14, 7.24e-14,
5.493e-14, 4.288e-14, 3.427e-14, 2.787e-14, 2.296e-14, 1.909e-14,
1.598e-14, 1.344e-14, 1.135e-14, 9.616e-15, 8.169e-15, 6.957e-15,
5.938e-15, 5.08e-15, 4.353e-15, 3.738e-15, 3.217e-15, 2.773e-15,
2.397e-15, 2.077e-15, 1.805e-15, 1.575e-15, 1.382e-15, 1.221e-15,
1.09e-15, 9.855e-16, 9.068e-16, 8.537e-16, 8.27e-16, 8.29e-16,
8.634e-16, 9.359e-16, 1.055e-15, 1.233e-15, 1.486e-15, 1.839e-15,
2.326e-15, 2.998e-15, 3.934e-15, 5.256e-15, 7.164e-15, 9.984e-15,
1.427e-14, 2.099e-14, 3.196e-14, 5.121e-14, 7.908e-14, 1.131e-13,
1.602e-13, 2.239e-13, 3.075e-13, 4.134e-13, 5.749e-13, 7.886e-13,
1.071e-12, 1.464e-12, 2.032e-12, 2.8e-12, 3.732e-12, 4.996e-12,
6.483e-12, 8.143e-12, 1.006e-11, 1.238e-11, 1.484e-11, 1.744e-11,
2.02e-11, 2.274e-11, 2.562e-11, 2.848e-11, 3.191e-11, 3.617e-11,
4.081e-11, 4.577e-11, 4.937e-11, 5.204e-11, 5.401e-11, 5.462e-11,
5.507e-11, 5.51e-11, 5.605e-11, 5.686e-11, 5.739e-11, 5.766e-11,
5.74e-11, 5.754e-11, 5.761e-11, 5.777e-11, 5.712e-11, 5.51e-11,
5.088e-11, 4.438e-11, 3.728e-11, 2.994e-11, 2.305e-11, 1.715e-11,
1.256e-11, 9.208e-12, 6.745e-12, 5.014e-12, 3.785e-12, 2.9e-12,
2.239e-12, 1.757e-12, 1.414e-12, 1.142e-12, 9.482e-13, 8.01e-13,
6.961e-13, 6.253e-13, 5.735e-13, 5.433e-13, 5.352e-13, 5.493e-13,
5.706e-13, 6.068e-13, 6.531e-13, 7.109e-13, 7.767e-13, 8.59e-13,
9.792e-13, 1.142e-12, 1.371e-12, 1.65e-12, 1.957e-12, 2.302e-12,
2.705e-12, 3.145e-12, 3.608e-12, 4.071e-12, 4.602e-12, 5.133e-12,
5.572e-12, 5.987e-12, 6.248e-12, 6.533e-12, 6.757e-12, 6.935e-12,
7.224e-12, 7.422e-12, 7.538e-12, 7.547e-12, 7.495e-12, 7.543e-12,
7.725e-12, 8.139e-12, 8.627e-12, 9.146e-12, 9.443e-12, 9.318e-12,
8.649e-12, 7.512e-12, 6.261e-12, 4.915e-12, 3.647e-12, 2.597e-12,
1.785e-12, 1.242e-12, 8.66e-13, 6.207e-13, 4.61e-13, 3.444e-13,
2.634e-13, 2.1e-13, 1.725e-13, 1.455e-13, 1.237e-13, 1.085e-13,
9.513e-14, 7.978e-14, 6.603e-14, 5.288e-14, 4.084e-14, 2.952e-14,
2.157e-14, 1.593e-14, 1.199e-14, 9.267e-15, 7.365e-15, 6.004e-15,
4.995e-15, 4.218e-15, 3.601e-15, 3.101e-15, 2.692e-15, 2.36e-15,
2.094e-15, 1.891e-15, 1.755e-15, 1.699e-15, 1.755e-15, 1.987e-15,
2.506e-15, 3.506e-15, 5.289e-15, 8.311e-15, 1.325e-14, 2.129e-14,
3.237e-14, 4.595e-14, 6.441e-14, 8.433e-14, 1.074e-13, 1.383e-13,
1.762e-13, 2.281e-13, 2.831e-13, 3.523e-13, 4.38e-13, 5.304e-13,
6.29e-13, 7.142e-13, 8.032e-13, 8.934e-13, 9.888e-13, 1.109e-12,
1.261e-12, 1.462e-12, 1.74e-12, 2.099e-12, 2.535e-12, 3.008e-12,
3.462e-12, 3.856e-12, 4.098e-12, 4.239e-12, 4.234e-12, 4.132e-12,
3.986e-12, 3.866e-12, 3.829e-12, 3.742e-12, 3.705e-12, 3.694e-12,
3.765e-12, 3.849e-12, 3.929e-12, 4.056e-12, 4.092e-12, 4.047e-12,
3.792e-12, 3.407e-12, 2.953e-12, 2.429e-12, 1.931e-12, 1.46e-12,
1.099e-12, 8.199e-13, 6.077e-13, 4.449e-13, 3.359e-13, 2.524e-13,
1.881e-13, 1.391e-13, 1.02e-13, 7.544e-14, 5.555e-14, 4.22e-14,
3.321e-14, 2.686e-14, 2.212e-14, 1.78e-14, 1.369e-14, 1.094e-14,
9.13e-15, 8.101e-15, 7.828e-15, 8.393e-15, 1.012e-14, 1.259e-14,
1.538e-14, 1.961e-14, 2.619e-14, 3.679e-14, 5.049e-14, 6.917e-14,
8.88e-14, 1.115e-13, 1.373e-13, 1.619e-13, 1.878e-13, 2.111e-13,
2.33e-13, 2.503e-13, 2.613e-13, 2.743e-13, 2.826e-13, 2.976e-13,
3.162e-13, 3.36e-13, 3.491e-13, 3.541e-13, 3.595e-13, 3.608e-13,
3.709e-13, 3.869e-13, 4.12e-13, 4.366e-13, 4.504e-13, 4.379e-13,
3.955e-13, 3.385e-13, 2.741e-13, 2.089e-13, 1.427e-13, 9.294e-14,
5.775e-14, 3.565e-14, 2.21e-14, 1.398e-14, 9.194e-15, 6.363e-15,
4.644e-15, 3.55e-15, 2.808e-15, 2.274e-15, 1.871e-15, 1.557e-15,
1.308e-15, 1.108e-15, 9.488e-16, 8.222e-16, 7.238e-16, 6.506e-16,
6.008e-16, 5.742e-16, 5.724e-16, 5.991e-16, 6.625e-16, 7.775e-16,
9.734e-16, 1.306e-15, 1.88e-15, 2.879e-15, 4.616e-15, 7.579e-15,
1.248e-14, 2.03e-14, 3.244e-14, 5.171e-14, 7.394e-14, 9.676e-14,
1.199e-13, 1.467e-13, 1.737e-13, 2.02e-13, 2.425e-13, 3.016e-13,
3.7e-13, 4.617e-13, 5.949e-13, 7.473e-13, 9.378e-13, 1.191e-12,
1.481e-12, 1.813e-12, 2.232e-12, 2.722e-12, 3.254e-12, 3.845e-12,
4.458e-12, 5.048e-12, 5.511e-12, 5.898e-12, 6.204e-12, 6.293e-12,
6.386e-12, 6.467e-12, 6.507e-12, 6.466e-12, 6.443e-12, 6.598e-12,
6.873e-12, 7.3e-12, 7.816e-12, 8.368e-12, 8.643e-12, 8.466e-12,
```

```
    7.871e-12, 6.853e-12, 5.714e-12, 4.482e-12, 3.392e-12, 2.613e-12,
    2.008e-12, 1.562e-12, 1.228e-12, 9.888e-13, 7.646e-13, 5.769e-13,
    4.368e-13, 3.324e-13, 2.508e-13, 1.916e-13
  };

  static double xfcrev[15] =
    { 1.003, 1.009, 1.015, 1.023, 1.029, 1.033, 1.037,
    1.039, 1.04, 1.046, 1.036, 1.027, 1.01, 1.002, 1.
  };

  double sfac;

  /* Get H2O continuum absorption... */
  double xw = nu / 10 + 1;
  if (xw >= 1 && xw < 2001) {
    int iw = (int) xw;
    double dw = xw - iw;
    double ew = 1 - dw;
    double cw296 = ew * h2o296[iw - 1] + dw * h2o296[iw];
    double cw260 = ew * h2o260[iw - 1] + dw * h2o260[iw];
    double cwfrn = ew * h2ofrn[iw - 1] + dw * h2ofrn[iw];
    if (nu <= 820 || nu >= 960) {
      sfac = 1;
    } else {
      double xx = (nu - 820) / 10;
      int ix = (int) xx;
      double dx = xx - ix;
      sfac = (1 - dx) * xfcrev[ix] + dx * xfcrev[ix + 1];
    }
    double ctwslf =
      sfac * cw296 * pow(cw260 / cw296, (296 - t) / (296 - 260));
    double vf2 = POW2(nu - 370);
    double vf6 = POW3(vf2);
    double fscal = 36100 / (vf2 + vf6 * 1e-8 + 36100) * -.25 + 1;
    double ctwfrn = cwfrn * fscal;
    double a1 = nu * u * tanh(.7193876 / t * nu);
    double a2 = 296 / t;
    double a3 = p / P0 * (q * ctwslf + (1 - q) * ctwfrn) * 1e-20;
    return a1 * a2 * a3;
  } else
    return 0;
}
```

5.19.3.8 ctmn2()

```
double ctmn2 (
        double nu,
        double p,
        double t )
```

Compute nitrogen continuum (absorption coefficient).

Definition at line 2805 of file jurassic.c.

```
                {

  static double ba[98] = { 0., 4.45e-8, 5.22e-8, 6.46e-8, 7.75e-8, 9.03e-8,
    1.06e-7, 1.21e-7, 1.37e-7, 1.57e-7, 1.75e-7, 2.01e-7, 2.3e-7,
    2.59e-7, 2.95e-7, 3.26e-7, 3.66e-7, 4.05e-7, 4.47e-7, 4.92e-7,
    5.34e-7, 5.84e-7, 6.24e-7, 6.67e-7, 7.14e-7, 7.26e-7, 7.54e-7,
    7.84e-7, 8.09e-7, 8.42e-7, 8.62e-7, 8.87e-7, 9.11e-7, 9.36e-7,
    9.76e-7, 1.03e-6, 1.11e-6, 1.23e-6, 1.39e-6, 1.61e-6, 1.76e-6,
    1.94e-6, 1.97e-6, 1.87e-6, 1.75e-6, 1.56e-6, 1.42e-6, 1.35e-6,
    1.32e-6, 1.29e-6, 1.29e-6, 1.29e-6, 1.3e-6, 1.32e-6, 1.33e-6,
    1.34e-6, 1.35e-6, 1.33e-6, 1.31e-6, 1.29e-6, 1.24e-6, 1.2e-6,
    1.16e-6, 1.1e-6, 1.04e-6, 9.96e-7, 9.38e-7, 8.63e-7, 7.98e-7,
    7.26e-7, 6.55e-7, 5.94e-7, 5.35e-7, 4.74e-7, 4.24e-7, 3.77e-7,
    3.33e-7, 2.96e-7, 2.63e-7, 2.34e-7, 2.08e-7, 1.85e-7, 1.67e-7,
    1.47e-7, 1.32e-7, 1.2e-7, 1.09e-7, 9.85e-8, 9.08e-8, 8.18e-8,
    7.56e-8, 6.85e-8, 6.14e-8, 5.83e-8, 5.77e-8, 5e-8, 4.32e-8, 0.
  };

  static double betaa[98] = { 802., 802., 761., 722., 679., 646., 609., 562.,
    511., 472., 436., 406., 377., 355., 338., 319., 299., 278., 255.,
    233., 208., 184., 149., 107., 66., 25., -13., -49., -82., -104.,
    -119., -130., -139., -144., -146., -146., -147., -148., -150.,
    -153., -160., -169., -181., -189., -195., -200., -205., -209.,
    -211., -210., -210., -209., -205., -199., -190., -180., -168.,
    -157., -143., -126., -108., -89., -63., -32., 1., 35., 65., 95.,
    121., 141., 152., 161., 164., 164., 161., 155., 148., 143., 137.,
    133., 131., 133., 139., 150., 165., 187., 213., 248., 284., 321.,
```

```
    372., 449., 514., 569., 609., 642., 673., 673.
  };

  static double nua[98] = { 2120., 2125., 2130., 2135., 2140., 2145., 2150.,
    2155., 2160., 2165., 2170., 2175., 2180., 2185., 2190., 2195.,
    2200., 2205., 2210., 2215., 2220., 2225., 2230., 2235., 2240.,
    2245., 2250., 2255., 2260., 2265., 2270., 2275., 2280., 2285.,
    2290., 2295., 2300., 2305., 2310., 2315., 2320., 2325., 2330.,
    2335., 2340., 2345., 2350., 2355., 2360., 2365., 2370., 2375.,
    2380., 2385., 2390., 2395., 2400., 2405., 2410., 2415., 2420.,
    2425., 2430., 2435., 2440., 2445., 2450., 2455., 2460., 2465.,
    2470., 2475., 2480., 2485., 2490., 2495., 2500., 2505., 2510.,
    2515., 2520., 2525., 2530., 2535., 2540., 2545., 2550., 2555.,
    2560., 2565., 2570., 2575., 2580., 2585., 2590., 2595., 2600., 2605.
  };

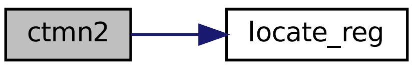
  const double q_n2 = 0.79, t0 = 273.0, tr = 296.0;

  /* Check wavenumber range... */
  if (nu < nua[0] || nu > nua[97])
    return 0;

  /* Interpolate B and beta... */
  int idx = locate_reg(nua, 98, nu);
  double b = LIN(nua[idx], ba[idx], nua[idx + 1], ba[idx + 1], nu);
  double beta = LIN(nua[idx], betaa[idx], nua[idx + 1], betaa[idx + 1], nu);

  /* Compute absorption coefficient... */
  return 0.1 * POW2(p / P0 * t0 / t) * exp(beta * (1 / tr - 1 / t))
    * q_n2 * b * (q_n2 + (1 - q_n2) * (1.294 - 0.4545 * t / tr));
}
```

Here is the call graph for this function:



5.19.3.9 ctmo2()

```
double ctmo2 (
    double nu,
    double p,
    double t )
```

Compute oxygen continuum (absorption coefficient).

Definition at line 2869 of file jurassic.c.

```
            {

  static double ba[90] = { 0., .061, .074, .084, .096, .12, .162, .208, .246,
    .285, .314, .38, .444, .5, .571, .673, .768, .853, .966, 1.097,
    1.214, 1.333, 1.466, 1.591, 1.693, 1.796, 1.922, 2.037, 2.154,
    2.264, 2.375, 2.508, 2.671, 2.847, 3.066, 3.417, 3.828, 4.204,
    4.453, 4.599, 4.528, 4.284, 3.955, 3.678, 3.477, 3.346, 3.29,
    3.251, 3.231, 3.226, 3.212, 3.192, 3.108, 3.033, 2.911, 2.798,
    2.646, 2.508, 2.322, 2.13, 1.928, 1.757, 1.588, 1.417, 1.253,
    1.109, .99, .888, .791, .678, .587, .524, .464, .403, .357, .32,
    .29, .267, .242, .215, .182, .16, .146, .128, .103, .087, .081,
    .071, .064, 0.
  };

  static double betaa[90] = { 467., 467., 400., 315., 379., 368., 475., 521.,
    531., 512., 442., 444., 430., 381., 335., 324., 296., 248., 215.,
    193., 158., 127., 101., 71., 31., -6., -26., -47., -63., -79.,
    -88., -88., -87., -90., -98., -99., -109., -134., -160., -167.,
```

```
    -164., -158., -153., -151., -156., -166., -168., -173., -170.,
    -161., -145., -126., -108., -84., -59., -29., 4., 41., 73., 97.,
    123., 159., 198., 220., 242., 256., 281., 311., 334., 319., 313.,
    321., 323., 310., 315., 320., 335., 361., 378., 373., 338., 319.,
    346., 322., 291., 290., 350., 371., 504., 504.
  };

  static double nua[90] = { 1360., 1365., 1370., 1375., 1380., 1385., 1390.,
    1395., 1400., 1405., 1410., 1415., 1420., 1425., 1430., 1435.,
    1440., 1445., 1450., 1455., 1460., 1465., 1470., 1475., 1480.,
    1485., 1490., 1495., 1500., 1505., 1510., 1515., 1520., 1525.,
    1530., 1535., 1540., 1545., 1550., 1555., 1560., 1565., 1570.,
    1575., 1580., 1585., 1590., 1595., 1600., 1605., 1610., 1615.,
    1620., 1625., 1630., 1635., 1640., 1645., 1650., 1655., 1660.,
    1665., 1670., 1675., 1680., 1685., 1690., 1695., 1700., 1705.,
    1710., 1715., 1720., 1725., 1730., 1735., 1740., 1745., 1750.,
    1755., 1760., 1765., 1770., 1775., 1780., 1785., 1790., 1795.,
    1800., 1805.
  };

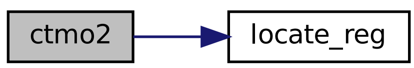
  const double q_o2 = 0.21, t0 = 273, tr = 296;

  /* Check wavenumber range... */
  if (nu < nua[0] || nu > nua[89])
    return 0;

  /* Interpolate B and beta... */
  int idx = locate_reg(nua, 90, nu);
  double b = LIN(nua[idx], ba[idx], nua[idx + 1], ba[idx + 1], nu);
  double beta = LIN(nua[idx], betaa[idx], nua[idx + 1], betaa[idx + 1], nu);

  /* Compute absorption coefficient... */
  return 0.1 * POW2(p / P0 * t0 / t) * exp(beta * (1 / tr - 1 / t)) * q_o2 *
    b;
}
```

Here is the call graph for this function:



5.19.3.10 copy_atm()

```
void copy_atm (
    ctl_t * ctl,
    atm_t * atm_dest,
    atm_t * atm_src,
    int init )
```

Copy and initialize atmospheric data.

Definition at line 2928 of file jurassic.c.

```
            {

  /* Data size... */
  size_t s = (size_t) atm_src->np * sizeof(double);

  /* Copy data... */
  atm_dest->np = atm_src->np;
  memcpy(atm_dest->time, atm_src->time, s);
  memcpy(atm_dest->z, atm_src->z, s);
  memcpy(atm_dest->lon, atm_src->lon, s);
  memcpy(atm_dest->lat, atm_src->lat, s);
  memcpy(atm_dest->p, atm_src->p, s);
  memcpy(atm_dest->t, atm_src->t, s);
```

```
  for (int ig = 0; ig < ctl->ng; ig++)
    memcpy(atm_dest->q[ig], atm_src->q[ig], s);
  for (int iw = 0; iw < ctl->nw; iw++)
    memcpy(atm_dest->k[iw], atm_src->k[iw], s);
  atm_dest->clz = atm_src->clz;
  atm_dest->cldz = atm_src->cldz;
  for (int icl = 0; icl < ctl->ncl; icl++)
    atm_dest->clk[icl] = atm_src->clk[icl];
  atm_dest->sfz = atm_src->sfz;
  atm_dest->sfp = atm_src->sfp;
  atm_dest->sft = atm_src->sft;
  for (int isf = 0; isf < ctl->nsf; isf++)
    atm_dest->sfeps[isf] = atm_src->sfeps[isf];

  /* Initialize... */
  if (init)
    for (int ip = 0; ip < atm_dest->np; ip++) {
      atm_dest->p[ip] = 0;
      atm_dest->t[ip] = 0;
      for (int ig = 0; ig < ctl->ng; ig++)
        atm_dest->q[ig][ip] = 0;
      for (int iw = 0; iw < ctl->nw; iw++)
        atm_dest->k[iw][ip] = 0;
      atm_dest->clz = 0;
      atm_dest->cldz = 0;
      for (int icl = 0; icl < ctl->ncl; icl++)
        atm_dest->clk[icl] = 0;
      atm_dest->sfz = 0;
      atm_dest->sfp = 0;
      atm_dest->sft = 0;
      for (int isf = 0; isf < ctl->nsf; isf++)
        atm_dest->sfeps[isf] = 1;
    }
}
```

5.19.3.11 copy_obs()

```
void copy_obs (
    ctl_t * ctl,
    obs_t * obs_dest,
    obs_t * obs_src,
    int init )
```

Copy and initialize observation data.

Definition at line 2982 of file jurassic.c.

```
            {

  /* Data size... */
  size_t s = (size_t) obs_src->nr * sizeof(double);

  /* Copy data... */
  obs_dest->nr = obs_src->nr;
  memcpy(obs_dest->time, obs_src->time, s);
  memcpy(obs_dest->obsz, obs_src->obsz, s);
  memcpy(obs_dest->obslon, obs_src->obslon, s);
  memcpy(obs_dest->obslat, obs_src->obslat, s);
  memcpy(obs_dest->vpz, obs_src->vpz, s);
  memcpy(obs_dest->vplon, obs_src->vplon, s);
  memcpy(obs_dest->vplat, obs_src->vplat, s);
  memcpy(obs_dest->tpz, obs_src->tpz, s);
  memcpy(obs_dest->tplon, obs_src->tplon, s);
  memcpy(obs_dest->tplat, obs_src->tplat, s);
  for (int id = 0; id < ctl->nd; id++)
    memcpy(obs_dest->rad[id], obs_src->rad[id], s);
  for (int id = 0; id < ctl->nd; id++)
    memcpy(obs_dest->tau[id], obs_src->tau[id], s);

  /* Initialize... */
  if (init)
    for (int id = 0; id < ctl->nd; id++)
      for (int ir = 0; ir < obs_dest->nr; ir++)
        if (gsl_finite(obs_dest->rad[id][ir])) {
          obs_dest->rad[id][ir] = 0;
          obs_dest->tau[id][ir] = 0;
        }
}
```

5.19.3.12 find_emitter()

```
int find_emitter (
    ctl_t * ctl,
    const char * emitter )
```

Find index of an emitter.

Definition at line 3020 of file jurassic.c.

```
                          {

  for (int ig = 0; ig < ctl->ng; ig++)
    if (strcasecmp(ctl->emitter[ig], emitter) == 0)
      return ig;

  return -1;
}
```

5.19.3.13 formod()

```
void formod (
    ctl_t * ctl,
    atm_t * atm,
    obs_t * obs )
```

Determine ray paths and compute radiative transfer.

Definition at line 3033 of file jurassic.c.

```
                  {

  int *mask;

  /* Allocate... */
  ALLOC(mask, int,
        ND * NR);

  /* Save observation mask... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ir = 0; ir < obs->nr; ir++)
      mask[id * NR + ir] = !gsl_finite(obs->rad[id][ir]);

  /* Hydrostatic equilibrium... */
  hydrostatic(ctl, atm);

  /* EGA forward model... */
  if (ctl->formod == 1)
    for (int ir = 0; ir < obs->nr; ir++)
      formod_pencil(ctl, atm, obs, ir);

  /* Call RFM... */
  else if (ctl->formod == 2)
    formod_rfm(ctl, atm, obs);

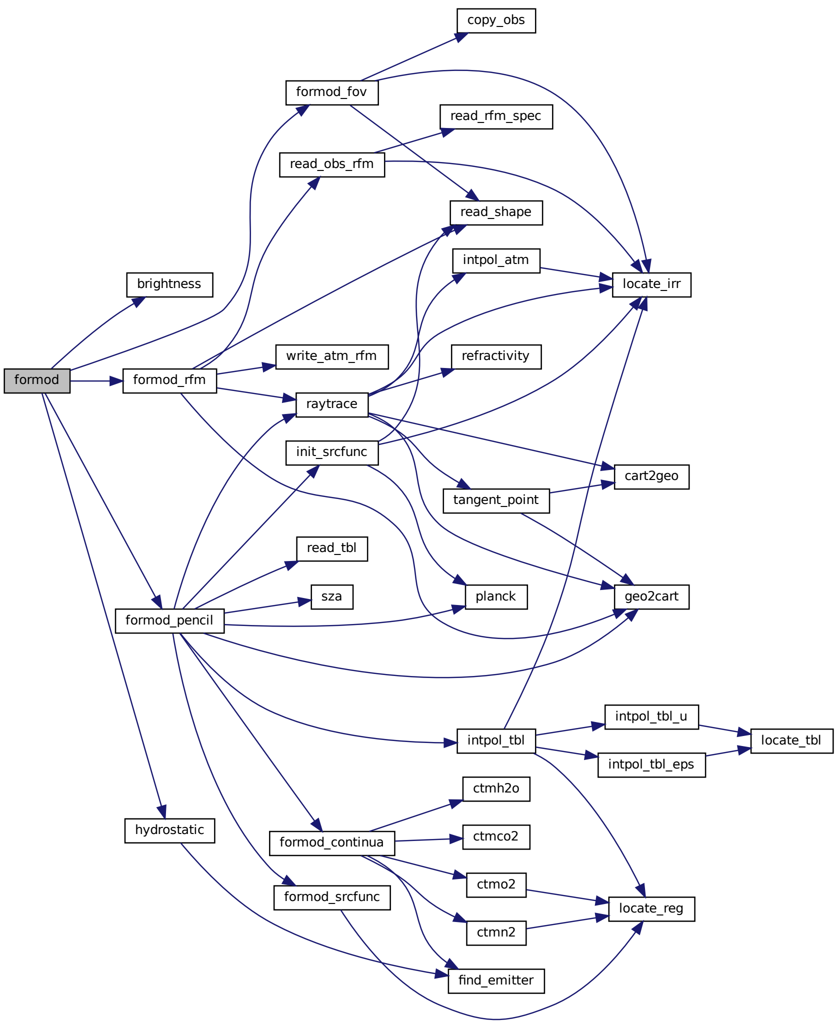
  /* Apply field-of-view convolution... */
  formod_fov(ctl, obs);

  /* Convert radiance to brightness temperature... */
  if (ctl->write_bbt)
    for (int id = 0; id < ctl->nd; id++)
      for (int ir = 0; ir < obs->nr; ir++)
        obs->rad[id][ir] = brightness(obs->rad[id][ir], ctl->nu[id]);

  /* Apply observation mask... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ir = 0; ir < obs->nr; ir++)
      if (mask[id * NR + ir])
        obs->rad[id][ir] = GSL_NAN;

  /* Free... */
  free(mask);
}
```

Here is the call graph for this function:



5.19.3.14 formod_continua() `void formod_continua ( ctl_t * ctl, los_t * los, int ip, double * beta )`

Compute absorption coefficient of continua.

Definition at line 3082 of file jurassic.c.

```
                         {

  static int ig_co2 = -999, ig_h2o = -999;

  /* Extinction... */
  for (int id = 0; id < ctl->nd; id++)
    beta[id] = los->k[ip][id];

  /* CO2 continuum... */
  if (ctl->ctm_co2) {
```

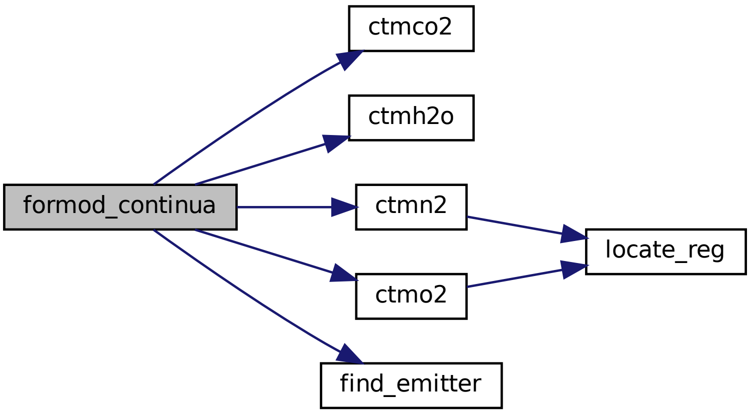
```
    if (ig_co2 == -999)
      ig_co2 = find_emitter(ctl, "CO2");
    if (ig_co2 >= 0)
      for (int id = 0; id < ctl->nd; id++)
        beta[id] += ctmco2(ctl->nu[id], los->p[ip], los->t[ip],
                           los->u[ip][ig_co2]) / los->ds[ip];
  }

  /* H2O continuum... */
  if (ctl->ctm_h2o) {
    if (ig_h2o == -999)
      ig_h2o = find_emitter(ctl, "H2O");
    if (ig_h2o >= 0)
      for (int id = 0; id < ctl->nd; id++)
        beta[id] += ctmh2o(ctl->nu[id], los->p[ip], los->t[ip],
                           los->q[ip][ig_h2o], los->u[ip][ig_h2o])
          / los->ds[ip];
  }

  /* N2 continuum... */
  if (ctl->ctm_n2)
    for (int id = 0; id < ctl->nd; id++)
      beta[id] += ctmn2(ctl->nu[id], los->p[ip], los->t[ip]);

  /* O2 continuum... */
  if (ctl->ctm_o2)
    for (int id = 0; id < ctl->nd; id++)
      beta[id] += ctmo2(ctl->nu[id], los->p[ip], los->t[ip]);
}
```

Here is the call graph for this function:



5.19.3.15 formod_fov() `void formod_fov ( ctl_t * ctl, obs_t * obs )`

Apply field of view convolution.

Definition at line 3128 of file jurassic.c.

```
03130                {
03131 
03132   static double dz[NSHAPE], w[NSHAPE];
03133 
03134   static int init = 0, n;
03135 
```

```
  obs_t *obs2;

  double rad[ND][NR], tau[ND][NR], z[NR];

  /* Do not take into account FOV... */
  if (ctl->fov[0] == '-')
    return;

  /* Initialize FOV data... */
  if (!init) {
    init = 1;
    read_shape(ctl->fov, dz, w, &n);
  }

  /* Allocate... */
  ALLOC(obs2, obs_t, 1);

  /* Copy observation data... */
  copy_obs(ctl, obs2, obs, 0);

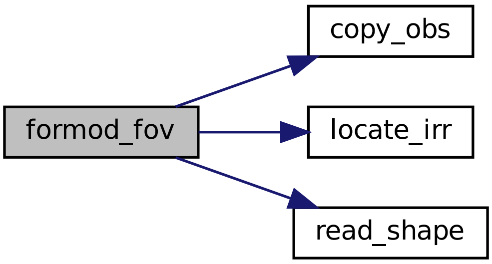
  /* Loop over ray paths... */
  for (int ir = 0; ir < obs->nr; ir++) {

    /* Get radiance and transmittance profiles... */
    int nz = 0;
    for (int ir2 = GSL_MAX(ir - NFOV, 0);
         ir2 < GSL_MIN(ir + 1 + NFOV, obs->nr); ir2++)
      if (obs->time[ir2] == obs->time[ir]) {
        z[nz] = obs2->vpz[ir2];
        for (int id = 0; id < ctl->nd; id++) {
          rad[id][nz] = obs2->rad[id][ir2];
          tau[id][nz] = obs2->tau[id][ir2];
        }
        nz++;
      }
    if (nz < 2)
      ERRMSG("Cannot apply FOV convolution!");

    /* Convolute profiles with FOV... */
    double wsum = 0;
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] = 0;
      obs->tau[id][ir] = 0;
    }
    for (int i = 0; i < n; i++) {
      double zfov = obs->vpz[ir] + dz[i];
      int idx = locate_irr(z, nz, zfov);
      for (int id = 0; id < ctl->nd; id++) {
        obs->rad[id][ir] += w[i]
          * LIN(z[idx], rad[id][idx], z[idx + 1], rad[id][idx + 1], zfov);
        obs->tau[id][ir] += w[i]
          * LIN(z[idx], tau[id][idx], z[idx + 1], tau[id][idx + 1], zfov);
      }
      wsum += w[i];
    }
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] /= wsum;
      obs->tau[id][ir] /= wsum;
    }
  }

  /* Free... */
  free(obs2);
}
```

Here is the call graph for this function:



5.19.3.16 formod_pencil()

```
void formod_pencil (
    ctl_t * ctl,
    atm_t * atm,
    obs_t * obs,
    int ir )
```

Compute radiative transfer for a pencil beam.

Definition at line 3203 of file jurassic.c.

```
                {

  static tbl_t *tbl;

  static int init = 0;

  los_t *los;

  double beta_ctm[ND], rad[ND], tau[ND], tau_refl[ND],
    tau_path[ND][NG], tau_gas[ND], x0[3], x1[3];

  /* Initialize look-up tables... */
  if (!init) {
    init = 1;
    ALLOC(tbl, tbl_t, 1);
    read_tbl(ctl, tbl);
    init_srcfunc(ctl, tbl);
  }

  /* Allocate... */
  ALLOC(los, los_t, 1);

  /* Initialize... */
  for (int id = 0; id < ctl->nd; id++) {
    rad[id] = 0;
    tau[id] = 1;
    for (int ig = 0; ig < ctl->ng; ig++)
      tau_path[id][ig] = 1;
  }

  /* Raytracing... */
  raytrace(ctl, atm, obs, los, ir);

  /* Loop over LOS points... */
  for (int ip = 0; ip < los->np; ip++) {

    /* Get trace gas transmittance... */
    intpol_tbl(ctl, tbl, los, ip, tau_path, tau_gas);

    /* Get continuum absorption... */
```

```
    formod_continua(ctl, los, ip, beta_ctm);

    /* Compute Planck function... */
    formod_srcfunc(ctl, tbl, los->t[ip], los->src[ip]);

    /* Loop over channels... */
    for (int id = 0; id < ctl->nd; id++)
      if (tau_gas[id] > 0) {

        /* Get segment emissivity... */
        los->eps[ip][id] = 1 - tau_gas[id] * exp(-beta_ctm[id] * los->ds[ip]);

        /* Compute radiance... */
        rad[id] += los->src[ip][id] * los->eps[ip][id] * tau[id];

        /* Compute path transmittance... */
        tau[id] *= (1 - los->eps[ip][id]);
      }
  }

  /* Check whether LOS hit the ground... */
  if (ctl->sftype >= 1 && los->sft > 0) {

    /* Add surface emissions... */
    double src_sf[ND];
    formod_srcfunc(ctl, tbl, los->sft, src_sf);
    for (int id = 0; id < ctl->nd; id++)
      rad[id] += los->sfeps[id] * src_sf[id] * tau[id];

    /* Check reflectivity... */
    int refl = 0;
    if (ctl->sftype >= 2)
      for (int id = 0; id < ctl->nd; id++)
        if (los->sfeps[id] < 1) {
          refl = 1;
          break;
        }

    /* Calculate reflection... */
    if (refl) {

      /* Initialize... */
      for (int id = 0; id < ctl->nd; id++)
        tau_refl[id] = 1;

      /* Add down-welling radiance... */
      for (int ip = los->np - 1; ip >= 0; ip--)
        for (int id = 0; id < ctl->nd; id++) {
          rad[id] += los->src[ip][id] * los->eps[ip][id] * tau_refl[id]
            * tau[id] * (1 - los->sfeps[id]);
          tau_refl[id] *= (1 - los->eps[ip][id]);
        }

      /* Add solar term... */
      if (ctl->sftype >= 3) {

        /* Get solar zenith angle... */
        double sza2;
        if (ctl->sfsza < 0)
          sza2 =
            sza(obs->time[ir], los->lon[los->np - 1], los->lat[los->np - 1]);
        else
          sza2 = ctl->sfsza;

        /* Check solar zenith angle... */
        if (sza2 < 89.999) {

          /* Get angle of incidence... */
          geo2cart(los->z[los->np - 1], los->lon[los->np - 1],
                   los->lat[los->np - 1], x0);
          geo2cart(los->z[0], los->lon[0], los->lat[0], x1);
          for (int i = 0; i < 3; i++)
            x1[i] -= x0[i];
          double cosa = DOTP(x0, x1) / NORM(x0) / NORM(x1);

          /* Get ratio of SZA and incident radiation... */
          double rcos = cosa / cos(sza2 * M_PI / 180.);

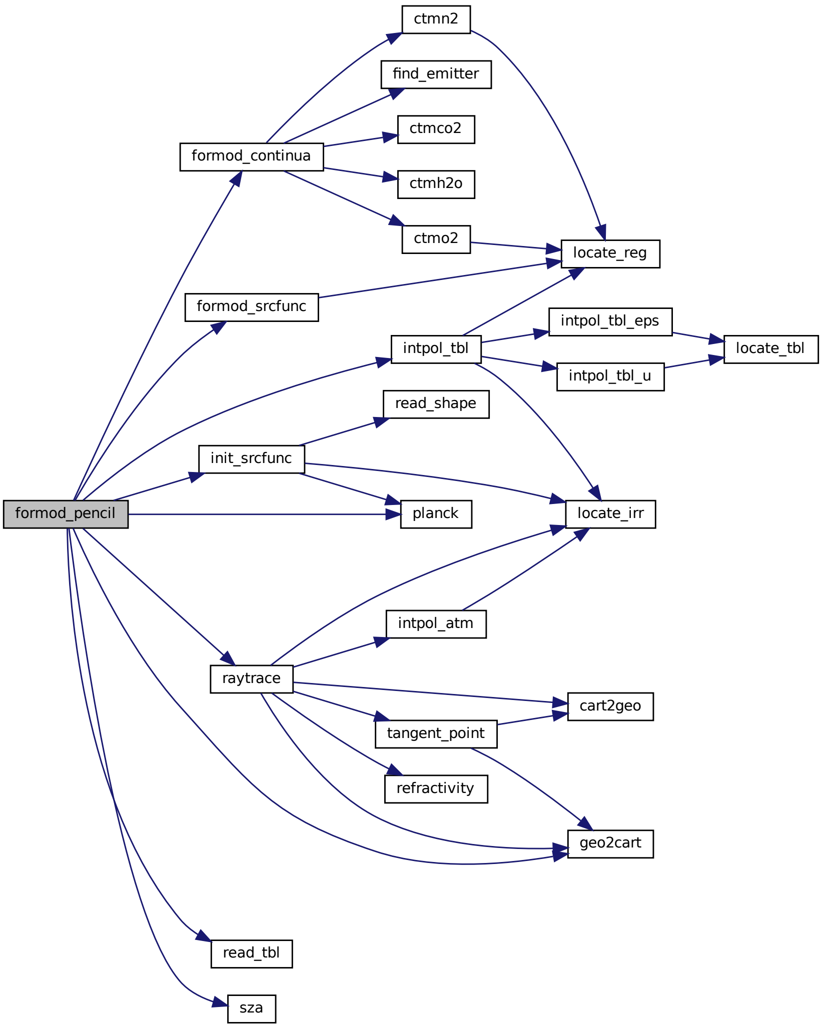
          /* Add solar radiation... */
          for (int id = 0; id < ctl->nd; id++)
            rad[id] += 6.764e-5 / (2. * M_PI) * planck(TSUN, ctl->nu[id])
              * tau_refl[id] * (1 - los->sfeps[id]) * tau[id] * rcos;
        }
      }
    }
  }

```

```
    /* Copy results... */
    for (int id = 0; id < ctl->nd; id++) {
      obs->rad[id][ir] = rad[id];
      obs->tau[id][ir] = tau[id];
    }

    /* Free... */
    free(los);
}
```

Here is the call graph for this function:



5.19.3.17 formod_rfm()

```
void formod_rfm (
    ctl_t * ctl,
    atm_t * atm,
    obs_t * obs )
```

Apply RFM for radiative transfer calculations.

Definition at line 3346 of file jurassic.c.

```
                {

los_t *los;

FILE *out;

char cmd[2 * LEN], filename[2 * LEN],
  rfmflg[LEN] = { "RAD TRA MIX LIN SFC" };

double f[NSHAPE], nu[NSHAPE], nu0, nu1, obsz = -999, tsurf,
  xd[3], xo[3], xv[3], z[NR], zmin, zmax;

int i, id, ig, ip, ir, iw, n, nadir = 0;

/* Allocate... */
ALLOC(los, los_t, 1);

/* Check observer positions... */
for (ir = 1; ir < obs->nr; ir++)
  if (obs->obsz[ir] != obs->obsz[0]
      || obs->obslon[ir] != obs->obslon[0]
      || obs->obslat[ir] != obs->obslat[0])
    ERRMSG("RFM interface requires identical observer positions!");

/* Check extinction data... */
for (iw = 0; iw < ctl->nw; iw++)
  for (ip = 0; ip < atm->np; ip++)
    if (atm->k[iw][ip] != 0)
      ERRMSG("RFM interface cannot handle extinction data!");

/* Get altitude range of atmospheric data... */
gsl_stats_minmax(&zmin, &zmax, atm->z, 1, (size_t) atm->np);

/* Observer within atmosphere? */
if (obs->obsz[0] >= zmin && obs->obsz[0] <= zmax) {
  obsz = obs->obsz[0];
  strcat(rfmflg, " OBS");
}

/* Determine tangent altitude or air mass factor... */
for (ir = 0; ir < obs->nr; ir++) {

  /* Raytracing... */
  raytrace(ctl, atm, obs, los, ir);

  /* Nadir? */
  if (obs->tpz[ir] <= zmin) {
    geo2cart(obs->obsz[ir], obs->obslon[ir], obs->obslat[ir], xo);
    geo2cart(obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], xv);
    for (i = 0; i < 3; i++)
      xd[i] = xo[i] - xv[i];
    z[ir] = NORM(xo) * NORM(xd) / DOTP(xo, xd);
    nadir++;
  } else
    z[ir] = obs->tpz[ir];
}
if (nadir > 0 && nadir < obs->nr)
  ERRMSG("Limb and nadir not simultaneously possible!");

/* Nadir? */
if (nadir)
  strcat(rfmflg, " NAD");

/* Get surface temperature... */
tsurf = atm->t[gsl_stats_min_index(atm->z, 1, (size_t) atm->np)];

/* Refraction? */
if (!nadir && !ctl->refrac)
  strcat(rfmflg, " GEO");

/* Continua? */
if (ctl->ctm_co2 || ctl->ctm_h2o || ctl->ctm_n2 || ctl->ctm_o2)
  strcat(rfmflg, " CTM");

/* Write atmospheric data file... */
write_atm_rfm("rfm.atm", ctl, atm);

/* Loop over channels... */
for (id = 0; id < ctl->nd; id++) {

  /* Read filter function... */
  sprintf(filename, "%s_%.4f.filt", ctl->tblbase, ctl->nu[id]);
  read_shape(filename, nu, f, &n);

  /* Set spectral range... */
  nu0 = nu[0];
  nu1 = nu[n - 1];
```

```

    /* Create RFM driver file... */
    if (!(out = fopen("rfm.drv", "w")))
      ERRMSG("Cannot create file!");
    fprintf(out, "*HDR\nRFM call by JURASSIC.\n");
    fprintf(out, "*FLG\n%s\n", rfmflg);
    fprintf(out, "*SPC\n%.4f %.4f 0.0005\n", nu0, nu1);
    fprintf(out, "*GAS\n");
    for (ig = 0; ig < ctl->ng; ig++)
      fprintf(out, "%s\n", ctl->emitter[ig]);
    fprintf(out, "*ATM\nrfm.atm\n");
    fprintf(out, "*TAN\n");
    for (ir = 0; ir < obs->nr; ir++)
      fprintf(out, "%g\n", z[ir]);
    fprintf(out, "*SFC\n%g 1.0\n", tsurf);
    if (obsz >= 0)
      fprintf(out, "*OBS\n%g\n", obsz);
    fprintf(out, "*HIT\n%s\n", ctl->rfmhit);
    fprintf(out, "*XSC\n");
    for (ig = 0; ig < ctl->ng; ig++)
      if (ctl->rfmxsc[ig][0] != '-')
        fprintf(out, "%s\n", ctl->rfmxsc[ig]);
    fprintf(out, "*END\n");
    fclose(out);

    /* Remove temporary files... */
    if (system("rm -f rfm.runlog rad_*.asc tra_*.asc"))
      ERRMSG("Cannot remove temporary files!");

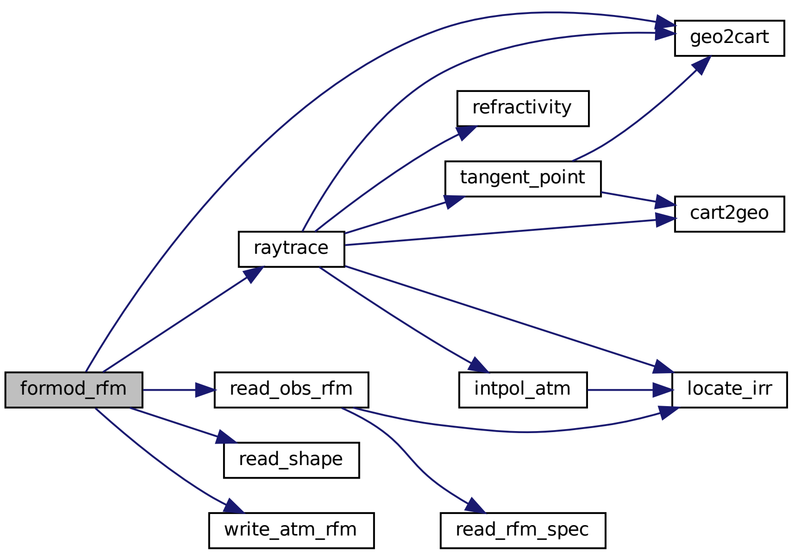
    /* Call RFM... */
    sprintf(cmd, "echo | %s", ctl->rfmbin);
    if (system(cmd))
      ERRMSG("Error while calling RFM!");

    /* Read data... */
    for (ir = 0; ir < obs->nr; ir++) {
      obs->rad[id][ir] = read_obs_rfm("rad", z[ir], nu, f, n) * 1e-5;
      obs->tau[id][ir] = read_obs_rfm("tra", z[ir], nu, f, n);
    }
  }

  /* Remove temporary files... */
  if (system("rm -f rfm.drv rfm.atm rfm.runlog rad_*.asc tra_*.asc"))
    ERRMSG("Error while removing temporary files!");

  /* Free... */
  free(los);
}
```

Here is the call graph for this function:



5.19.3.18 formod_srcfunc()

```
void formod_srcfunc (
    ctl_t * ctl,
    tbl_t * tbl,
    double t,
    double * src )
```

Compute Planck source function.

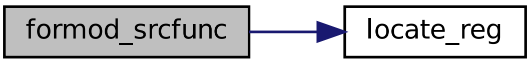
Definition at line 3487 of file jurassic.c.

```
                     {

  /* Determine index in temperature array... */
  int it = locate_reg(tbl->st, TBLNS, t);

  /* Interpolate Planck function value... */
  for (int id = 0; id < ctl->nd; id++)
    src[id] = LIN(tbl->st[it], tbl->sr[it][id],
                  tbl->st[it + 1], tbl->sr[it + 1][id], t);
}
```

Here is the call graph for this function:



5.19.3.19 geo2cart()

```
void geo2cart (
    double z,
    double lon,
    double lat,
    double * x )
```

Convert geolocation to Cartesian coordinates.

Definition at line 3504 of file jurassic.c.

```
                  {

  double radius = z + RE;

  x[0] = radius * cos(lat / 180 * M_PI) * cos(lon / 180 * M_PI);
  x[1] = radius * cos(lat / 180 * M_PI) * sin(lon / 180 * M_PI);
  x[2] = radius * sin(lat / 180 * M_PI);
}
```

5.19.3.20 hydrostatic() `void hydrostatic ( ctl_t * ctl, atm_t * atm )`

Set hydrostatic equilibrium.

Definition at line 3519 of file jurassic.c.

```
                     {

  const double mmair = 28.96456e-3, mmh2o = 18.0153e-3;

  const int ipts = 20;

  static int ig_h2o = -999;

  double dzmin = 1e99, e = 0;

  int ipref = 0;

  /* Check reference height... */
  if (ctl->hydz < 0)
    return;

  /* Determine emitter index of H2O... */
  if (ig_h2o == -999)
    ig_h2o = find_emitter(ctl, "H2O");

  /* Find air parcel next to reference height... */
  for (int ip = 0; ip < atm->np; ip++)
    if (fabs(atm->z[ip] - ctl->hydz) < dzmin) {
      dzmin = fabs(atm->z[ip] - ctl->hydz);
      ipref = ip;
    }

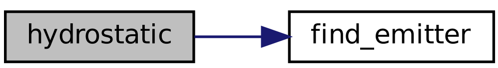
  /* Upper part of profile... */
  for (int ip = ipref + 1; ip < atm->np; ip++) {
    double mean = 0;
    for (int i = 0; i < ipts; i++) {
      if (ig_h2o >= 0)
        e = LIN(0.0, atm->q[ig_h2o][ip - 1],
                ipts - 1.0, atm->q[ig_h2o][ip], (double) i);
      mean += (e * mmh2o + (1 - e) * mmair)
        * G0 / RI
        / LIN(0.0, atm->t[ip - 1], ipts - 1.0, atm->t[ip], (double) i) / ipts;
    }

    /* Compute p(z,T)... */
    atm->p[ip] =
      exp(log(atm->p[ip - 1]) - mean * 1000 * (atm->z[ip] - atm->z[ip - 1]));
  }

  /* Lower part of profile... */
  for (int ip = ipref - 1; ip >= 0; ip--) {
    double mean = 0;
    for (int i = 0; i < ipts; i++) {
      if (ig_h2o >= 0)
        e = LIN(0.0, atm->q[ig_h2o][ip + 1],
                ipts - 1.0, atm->q[ig_h2o][ip], (double) i);
      mean += (e * mmh2o + (1 - e) * mmair)
        * G0 / RI
        / LIN(0.0, atm->t[ip + 1], ipts - 1.0, atm->t[ip], (double) i) / ipts;
    }

    /* Compute p(z,T)... */
    atm->p[ip] =
      exp(log(atm->p[ip + 1]) - mean * 1000 * (atm->z[ip] - atm->z[ip + 1]));
  }
}
```

Here is the call graph for this function:



5.19.3.21 idx2name()

```
void idx2name (
    ctl_t * ctl,
    int idx,
    char * quantity )
```

Determine name of state vector quantity for given index.

Definition at line 3585 of file jurassic.c.

```
                  {

  if (idx == IDXP)
    sprintf(quantity, "PRESSURE");

  if (idx == IDXT)
    sprintf(quantity, "TEMPERATURE");

  for (int ig = 0; ig < ctl->ng; ig++)
    if (idx == IDXQ(ig))
      sprintf(quantity, "%s", ctl->emitter[ig]);

  for (int iw = 0; iw < ctl->nw; iw++)
    if (idx == IDXK(iw))
      sprintf(quantity, "EXTINCT_WINDOW_%d", iw);

  if (idx == IDXCLZ)
    sprintf(quantity, "CLOUD_HEIGHT");

  if (idx == IDXCLDZ)
    sprintf(quantity, "CLOUD_DEPTH");

  for (int icl = 0; icl < ctl->ncl; icl++)
    if (idx == IDXCLK(icl))
      sprintf(quantity, "CLOUD_EXTINCT_%.4f", ctl->clnu[icl]);

  if (idx == IDXSFZ)
    sprintf(quantity, "SURFACE_HEIGHT");

  if (idx == IDXSFP)
    sprintf(quantity, "SURFACE_PRESSURE");

  if (idx == IDXSFT)
    sprintf(quantity, "SURFACE_TEMPERATURE");

  for (int isf = 0; isf < ctl->nsf; isf++)
    if (idx == IDXSFEPS(isf))
      sprintf(quantity, "SURFACE_EMISSIVITY_%.4f", ctl->sfnu[isf]);
}
```

5.19.3.22 init_srcfunc()

```
void init_srcfunc (
    ctl_t * ctl,
    tbl_t * tbl )
```

Initialize source function table.

Definition at line 3630 of file jurassic.c.

```
               {

  char filename[2 * LEN];

  double f[NSHAPE], nu[NSHAPE];

  int n;

  /* Write info... */
  LOG(1, "Initialize source function table...");

  /* Loop over channels... */
  for (int id = 0; id < ctl->nd; id++) {

    /* Read filter function... */
```

```
    sprintf(filename, "%s_%.4f.filt", ctl->tblbase, ctl->nu[id]);
    read_shape(filename, nu, f, &n);

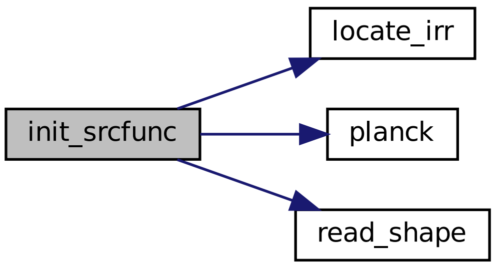
    /* Get minimum grid spacing... */
    double dnu = 1.0;
    for (int i = 1; i < n; i++)
      dnu = GSL_MIN(dnu, nu[i] - nu[i - 1]);

    /* Compute source function table... */
#pragma omp parallel for default(none) shared(ctl,tbl,id,nu,f,n,dnu)
    for (int it = 0; it < TBLNS; it++) {

      /* Set temperature... */
      tbl->st[it] = LIN(0.0, TMIN, TBLNS - 1.0, TMAX, (double) it);

      /* Integrate Planck function... */
      double fsum = tbl->sr[it][id] = 0;
      for (double fnu = nu[0]; fnu <= nu[n - 1]; fnu += dnu) {
        int i = locate_irr(nu, n, fnu);
        double ff = LIN(nu[i], f[i], nu[i + 1], f[i + 1], fnu);
        fsum += ff;
        tbl->sr[it][id] += ff * planck(tbl->st[it], fnu);
      }
      tbl->sr[it][id] /= fsum;
    }
  }
}
```

Here is the call graph for this function:



5.19.3.23 intpol_atm()

```
void intpol_atm (
    ctl_t * ctl,
    atm_t * atm,
    double z,
    double * p,
    double * t,
    double * q,
    double * k )
```

Interpolate atmospheric data.

Definition at line 3677 of file jurassic.c.

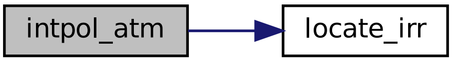
```
             {

  /* Get array index... */
  int ip = locate_irr(atm->z, atm->np, z);

  /* Interpolate... */
  *p = EXP(atm->z[ip], atm->p[ip], atm->z[ip + 1], atm->p[ip + 1], z);
```

```
  *t = LIN(atm->z[ip], atm->t[ip], atm->z[ip + 1], atm->t[ip + 1], z);
  for (int ig = 0; ig < ctl->ng; ig++)
    q[ig] =
      LIN(atm->z[ip], atm->q[ig][ip], atm->z[ip + 1], atm->q[ig][ip + 1], z);
  for (int iw = 0; iw < ctl->nw; iw++)
    k[iw] =
      LIN(atm->z[ip], atm->k[iw][ip], atm->z[ip + 1], atm->k[iw][ip + 1], z);
}
```

Here is the call graph for this function:



5.19.3.24 intpol_tbl()

```
void intpol_tbl (
    ctl_t * ctl,
    tbl_t * tbl,
    los_t * los,
    int ip,
    double tau_path[ND][NG],
    double tau_seg[ND] )
```

Get transmittance from look-up tables.

Definition at line 3702 of file jurassic.c.

```
                          {

  double eps, u;

  /* Loop over channels... */
  for (int id = 0; id < ctl->nd; id++) {

    /* Initialize... */
    tau_seg[id] = 1;

    /* Loop over emitters.... */
    for (int ig = 0; ig < ctl->ng; ig++) {

      /* Check size of table (pressure)... */
      if (tbl->np[id][ig] < 30)
        eps = 0;

      /* Check transmittance... */
      else if (tau_path[id][ig] < 1e-9)
        eps = 1;

      /* Interpolate... */
      else {

        /* Determine pressure and temperature indices... */
        int ipr = locate_irr(tbl->p[id][ig], tbl->np[id][ig], los->p[ip]);
        int it0 =
          locate_reg(tbl->t[id][ig][ipr], tbl->nt[id][ig][ipr], los->t[ip]);
        int it1 =
          locate_reg(tbl->t[id][ig][ipr + 1], tbl->nt[id][ig][ipr + 1],
                     los->t[ip]);

        /* Check size of table (temperature and column density)... */
        if (tbl->nt[id][ig][ipr] < 2 || tbl->nt[id][ig][ipr + 1] < 2
            || tbl->nu[id][ig][ipr][it0] < 2
            || tbl->nu[id][ig][ipr][it0 + 1] < 2
            || tbl->nu[id][ig][ipr + 1][it1] < 2
```

```
          || tbl->nu[id][ig][ipr + 1][it1 + 1] < 2)
        eps = 0;

      else {

        /* Get emissivities of extended path... */
        u = intpol_tbl_u(tbl, ig, id, ipr, it0, 1 - tau_path[id][ig]);
        double eps00
          = intpol_tbl_eps(tbl, ig, id, ipr, it0, u + los->u[ip][ig]);

        u = intpol_tbl_u(tbl, ig, id, ipr, it0 + 1, 1 - tau_path[id][ig]);
        double eps01 =
          intpol_tbl_eps(tbl, ig, id, ipr, it0 + 1, u + los->u[ip][ig]);

        u = intpol_tbl_u(tbl, ig, id, ipr + 1, it1, 1 - tau_path[id][ig]);
        double eps10 =
          intpol_tbl_eps(tbl, ig, id, ipr + 1, it1, u + los->u[ip][ig]);

        u =
          intpol_tbl_u(tbl, ig, id, ipr + 1, it1 + 1, 1 - tau_path[id][ig]);
        double eps11 =
          intpol_tbl_eps(tbl, ig, id, ipr + 1, it1 + 1, u + los->u[ip][ig]);

        /* Interpolate with respect to temperature... */
        eps00 = LIN(tbl->t[id][ig][ipr][it0], eps00,
                    tbl->t[id][ig][ipr][it0 + 1], eps01, los->t[ip]);
        eps11 = LIN(tbl->t[id][ig][ipr + 1][it1], eps10,
                    tbl->t[id][ig][ipr + 1][it1 + 1], eps11, los->t[ip]);

        /* Interpolate with respect to pressure... */
        eps00 = LIN(tbl->p[id][ig][ipr], eps00,
                    tbl->p[id][ig][ipr + 1], eps11, los->p[ip]);

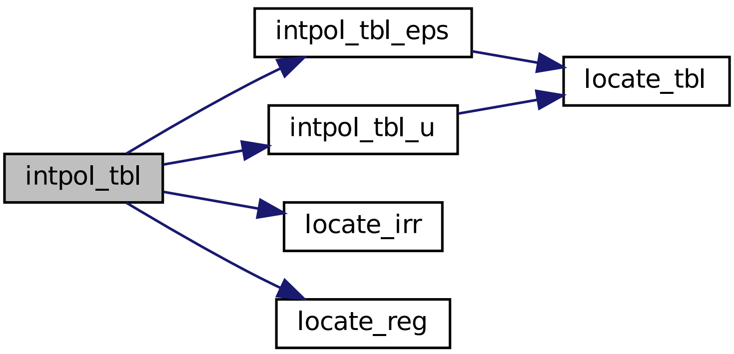
        /* Check emssivity range... */
        eps00 = GSL_MAX(GSL_MIN(eps00, 1), 0);

        /* Determine segment emissivity... */
        eps = 1 - (1 - eps00) / tau_path[id][ig];
      }
    }

    /* Get transmittance of extended path... */
    tau_path[id][ig] *= (1 - eps);

    /* Get segment transmittance... */
    tau_seg[id] *= (1 - eps);
  }
 }
}
```

Here is the call graph for this function:



5.19.3.25 intpol_tbl_eps()

```
double intpol_tbl_eps (
        tbl_t * tbl,
        int ig,
        int id,
        int ip,
        int it,
        double u )
```

Interpolate emissivity from look-up tables.

Definition at line 3797 of file jurassic.c.

```
              {

  /* Lower boundary... */
  if (u < tbl->u[id][ig][ip][it][0])
    return LIN(0, 0, tbl->u[id][ig][ip][it][0], tbl->eps[id][ig][ip][it][0],
               u);

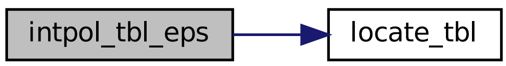
  /* Upper boundary... */
  else if (u > tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1])
    return LIN(tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               1e30, 1, u);

  /* Interpolation... */
  else {

    /* Get index... */
    int idx = locate_tbl(tbl->u[id][ig][ip][it], tbl->nu[id][ig][ip][it], u);

    /* Interpolate... */
    return
      LIN(tbl->u[id][ig][ip][it][idx], tbl->eps[id][ig][ip][it][idx],
          tbl->u[id][ig][ip][it][idx + 1], tbl->eps[id][ig][ip][it][idx + 1],
          u);
  }
}
```

Here is the call graph for this function:



5.19.3.26 intpol_tbl_u()

```
double intpol_tbl_u (
        tbl_t * tbl,
        int ig,
        int id,
        int ip,
        int it,
        double eps )
```

Interpolate column density from look-up tables.

Definition at line 3832 of file jurassic.c.

```
                {

  /* Lower boundary... */
```

```
  if (eps < tbl->eps[id][ig][ip][it][0])
    return LIN(0, 0, tbl->eps[id][ig][ip][it][0], tbl->u[id][ig][ip][it][0],
               eps);

  /* Upper boundary... */
  else if (eps > tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1])
    return LIN(tbl->eps[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               tbl->u[id][ig][ip][it][tbl->nu[id][ig][ip][it] - 1],
               1, 1e30, eps);

  /* Interpolation... */
  else {

    /* Get index... */
    int idx
      = locate_tbl(tbl->eps[id][ig][ip][it], tbl->nu[id][ig][ip][it], eps);

    /* Interpolate... */
    return
      LIN(tbl->eps[id][ig][ip][it][idx], tbl->u[id][ig][ip][it][idx],
          tbl->eps[id][ig][ip][it][idx + 1], tbl->u[id][ig][ip][it][idx + 1],
          eps);
  }
}
```

Here is the call graph for this function:

5.19.3.27 jsec2time()

```
void jsec2time (
        double jsec,
        int * year,
        int * mon,
        int * day,
        int * hour,
        int * min,
        int * sec,
        double * remain )
```

Convert seconds to date.

Definition at line 3868 of file jurassic.c.

```
                       {

  struct tm t0, *t1;

  t0.tm_year = 100;
  t0.tm_mon = 0;
  t0.tm_mday = 1;
  t0.tm_hour = 0;
  t0.tm_min = 0;
  t0.tm_sec = 0;

  time_t jsec0 = (time_t) jsec + timegm(&t0);
  t1 = gmtime(&jsec0);

  *year = t1->tm_year + 1900;
  *mon = t1->tm_mon + 1;
  *day = t1->tm_mday;
  *hour = t1->tm_hour;
```

```
  *min = t1->tm_min;
  *sec = t1->tm_sec;
  *remain = jsec - floor(jsec);
}
```

5.19.3.28 kernel()

```
void kernel (
    ctl_t * ctl,
    atm_t * atm,
    obs_t * obs,
    gsl_matrix * k )
```

Compute Jacobians.

Definition at line 3901 of file jurassic.c.

```
                    {

  atm_t *atm1;
  obs_t *obs1;

  gsl_vector *x0, *x1, *yy0, *yy1;

  int *iqa;

  /* Get sizes... */
  size_t m = k->size1;
  size_t n = k->size2;

  /* Allocate... */
  x0 = gsl_vector_alloc(n);
  yy0 = gsl_vector_alloc(m);
  ALLOC(iqa, int,
        N);

  /* Compute radiance for undisturbed atmospheric data... */
  formod(ctl, atm, obs);

  /* Compose vectors... */
  atm2x(ctl, atm, x0, iqa, NULL);
  obs2y(ctl, obs, yy0, NULL, NULL);

  /* Initialize kernel matrix... */
  gsl_matrix_set_zero(k);

  /* Loop over state vector elements... */
#pragma omp parallel for default(none) shared(ctl,atm,obs,k,x0,yy0,n,m,iqa) private(x1, yy1, atm1,
 obs1)
  for (size_t j = 0; j < n; j++) {

    /* Allocate... */
    x1 = gsl_vector_alloc(n);
    yy1 = gsl_vector_alloc(m);
    ALLOC(atm1, atm_t, 1);
    ALLOC(obs1, obs_t, 1);

    /* Set perturbation size... */
    double h;
    if (iqa[j] == IDXP)
      h = GSL_MAX(fabs(0.01 * gsl_vector_get(x0, j)), 1e-7);
    else if (iqa[j] == IDXT)
      h = 1.0;
    else if (iqa[j] >= IDXQ(0) && iqa[j] < IDXQ(ctl->ng))
      h = GSL_MAX(fabs(0.01 * gsl_vector_get(x0, j)), 1e-15);
    else if (iqa[j] >= IDXK(0) && iqa[j] < IDXK(ctl->nw))
      h = 1e-4;
    else if (iqa[j] == IDXCLZ || iqa[j] == IDXCLDZ)
      h = 1.0;
    else if (iqa[j] >= IDXCLK(0) && iqa[j] < IDXCLK(ctl->ncl))
      h = 1e-4;
    else if (iqa[j] == IDXSFZ)
      h = 0.1;
    else if (iqa[j] == IDXSFP)
      h = 10.0;
    else if (iqa[j] == IDXSFT)
      h = 1.0;
    else if (iqa[j] >= IDXSFEPS(0) && iqa[j] < IDXSFEPS(ctl->nsf))
      h = 1e-2;
    else
```

```
      ERRMSG("Cannot set perturbation size!");

    /* Disturb state vector element... */
    gsl_vector_memcpy(x1, x0);
    gsl_vector_set(x1, j, gsl_vector_get(x1, j) + h);
    copy_atm(ctl, atm1, atm, 0);
    copy_obs(ctl, obs1, obs, 0);
    x2atm(ctl, x1, atm1);

    /* Compute radiance for disturbed atmospheric data... */
    formod(ctl, atm1, obs1);

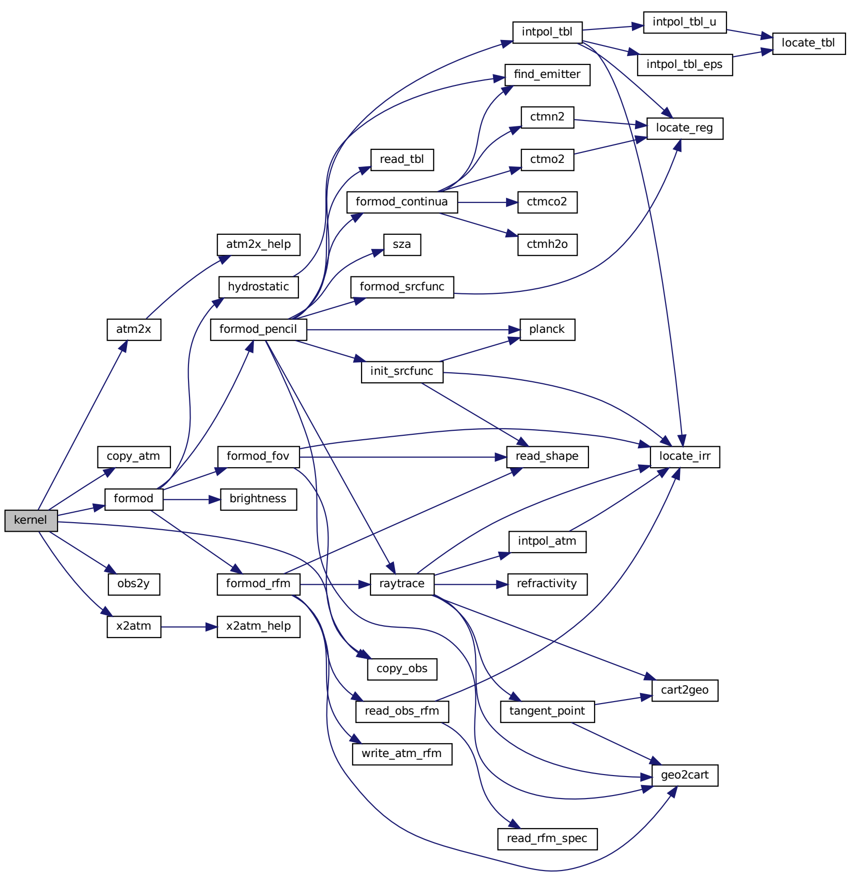
    /* Compose measurement vector for disturbed radiance data... */
    obs2y(ctl, obs1, yy1, NULL, NULL);

    /* Compute derivatives... */
    for (size_t i = 0; i < m; i++)
      gsl_matrix_set(k, i, j,
                     (gsl_vector_get(yy1, i) - gsl_vector_get(yy0, i)) / h);

    /* Free... */
    gsl_vector_free(x1);
    gsl_vector_free(yy1);
    free(atm1);
    free(obs1);
  }

  /* Free... */
  gsl_vector_free(x0);
  gsl_vector_free(yy0);
  free(iqa);
}
```

Here is the call graph for this function:



5.19.3.29 locate_irr()

```
int locate_irr (
    double * xx,
    int n,
    double x )
```

Find array index for irregular grid.

Definition at line 4002 of file jurassic.c.

```
                {

  int ilo = 0;
  int ihi = n - 1;
  int i = (ihi + ilo) » 1;

  if (xx[i] < xx[i + 1])
    while (ihi > ilo + 1) {
      i = (ihi + ilo) » 1;
      if (xx[i] > x)
        ihi = i;
      else
        ilo = i;
  } else
    while (ihi > ilo + 1) {
      i = (ihi + ilo) » 1;
      if (xx[i] <= x)
        ihi = i;
      else
        ilo = i;
    }

  return ilo;
}
```

5.19.3.30 locate_reg()

```
int locate_reg (
    double * xx,
    int n,
    double x )
```

Find array index for regular grid.

Definition at line 4032 of file jurassic.c.

```
                {

  /* Calculate index... */
  int i = (int) ((x - xx[0]) / (xx[1] - xx[0]));

  /* Check range... */
  if (i < 0)
    return 0;
  else if (i > n - 2)
    return n - 2;
  else
    return i;
}
```

5.19.3.31 locate_tbl()

```
int locate_tbl (
    float * xx,
    int n,
    double x )
```

Find array index in float array.

Definition at line 4051 of file jurassic.c.

```
                {

  int ilo = 0;
```

```
  int ihi = n - 1;
  int i = (ihi + ilo) » 1;

  while (ihi > ilo + 1) {
    i = (ihi + ilo) » 1;
    if (xx[i] > x)
      ihi = i;
    else
      ilo = i;
  }

  return ilo;
}
```

5.19.3.32 obs2y()

```
size_t obs2y (
    ctl_t * ctl,
    obs_t * obs,
    gsl_vector * y,
    int * ida,
    int * ira )
```

Compose measurement vector.

Definition at line 4073 of file jurassic.c.

```
                {

  size_t m = 0;

  /* Determine measurement vector... */
  for (int ir = 0; ir < obs->nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      if (gsl_finite(obs->rad[id][ir])) {
        if (y != NULL)
          gsl_vector_set(y, m, obs->rad[id][ir]);
        if (ida != NULL)
          ida[m] = id;
        if (ira != NULL)
          ira[m] = ir;
        m++;
      }

  return m;
}
```

5.19.3.33 planck()

```
double planck (
    double t,
    double nu )
```

Compute Planck function.

Definition at line 4100 of file jurassic.c.

```
                {

  return C1 * POW3(nu) / gsl_expm1(C2 * nu / t);
}
```

5.19.3.34 raytrace()

```
void raytrace (
        ctl_t * ctl,
        atm_t * atm,
        obs_t * obs,
        los_t * los,
        int ir )
```

Do ray-tracing to determine LOS.

Definition at line 4109 of file jurassic.c.

```
                {

  const double h = 0.02, zrefrac = 60;

  double ds, ex0[3], ex1[3], k[NW], lat, lon, n, ng[3], norm,
    p, q[NG], t, x[3], xh[3], xobs[3], xvp[3], z = 1e99, zmax, zmin;

  int stop = 0;

  /* Initialize... */
  los->np = 0;
  los->sft = -999;
  obs->tpz[ir] = obs->vpz[ir];
  obs->tplon[ir] = obs->vplon[ir];
  obs->tplat[ir] = obs->vplat[ir];

  /* Get altitude range of atmospheric data... */
  gsl_stats_minmax(&zmin, &zmax, atm->z, 1, (size_t) atm->np);
  if (ctl->nsf > 0) {
    zmin = GSL_MAX(atm->sfz, zmin);
    if (atm->sfp > 0) {
      int ip = locate_irr(atm->p, atm->np, atm->sfp);
      double zip = LIN(log(atm->p[ip]), atm->z[ip],
                       log(atm->p[ip + 1]), atm->z[ip + 1], log(atm->sfp));
      zmin = GSL_MAX(zip, zmin);
    }
  }

  /* Check observer altitude... */
  if (obs->obsz[ir] < zmin)
    ERRMSG("Observer below surface!");

  /* Check view point altitude... */
  if (obs->vpz[ir] > zmax)
    return;

  /* Determine Cartesian coordinates for observer and view point... */
  geo2cart(obs->obsz[ir], obs->obslon[ir], obs->obslat[ir], xobs);
  geo2cart(obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], xvp);

  /* Determine initial tangent vector... */
  for (int i = 0; i < 3; i++)
    ex0[i] = xvp[i] - xobs[i];
  norm = NORM(ex0);
  for (int i = 0; i < 3; i++)
    ex0[i] /= norm;

  /* Observer within atmosphere... */
  for (int i = 0; i < 3; i++)
    x[i] = xobs[i];

  /* Observer above atmosphere (search entry point)... */
  if (obs->obsz[ir] > zmax) {
    double dmax = norm, dmin = 0;
    while (fabs(dmin - dmax) > 0.001) {
      double d = (dmax + dmin) / 2;
      for (int i = 0; i < 3; i++)
        x[i] = xobs[i] + d * ex0[i];
      cart2geo(x, &z, &lon, &lat);
      if (z <= zmax && z > zmax - 0.001)
        break;
      if (z < zmax - 0.0005)
        dmax = d;
      else
        dmin = d;
    }
  }

  /* Ray-tracing... */
  while (1) {

    /* Set step length... */
    ds = ctl->rayds;
```

```
    if (ctl->raydz > 0) {
      norm = NORM(x);
      for (int i = 0; i < 3; i++)
        xh[i] = x[i] / norm;
      double cosa = fabs(DOTP(ex0, xh));
      if (cosa != 0)
        ds = GSL_MIN(ctl->rayds, ctl->raydz / cosa);
    }

    /* Determine geolocation... */
    cart2geo(x, &z, &lon, &lat);

    /* Check if LOS hits the ground or has left atmosphere... */
    if (z < zmin || z > zmax) {
      stop = (z < zmin ? 2 : 1);
      double frac =
        ((z <
          zmin ? zmin : zmax) - los->z[los->np - 1]) / (z - los->z[los->np -
                                                                    1]);
      geo2cart(los->z[los->np - 1], los->lon[los->np - 1],
               los->lat[los->np - 1], xh);
      for (int i = 0; i < 3; i++)
        x[i] = xh[i] + frac * (x[i] - xh[i]);
      cart2geo(x, &z, &lon, &lat);
      los->ds[los->np - 1] = ds * frac;
      ds = 0;
    }

    /* Interpolate atmospheric data... */
    intpol_atm(ctl, atm, z, &p, &t, q, k);

    /* Save data... */
    los->lon[los->np] = lon;
    los->lat[los->np] = lat;
    los->z[los->np] = z;
    los->p[los->np] = p;
    los->t[los->np] = t;
    for (int ig = 0; ig < ctl->ng; ig++)
      los->q[los->np][ig] = q[ig];
    for (int id = 0; id < ctl->nd; id++)
      los->k[los->np][id] = k[ctl->window[id]];
    los->ds[los->np] = ds;

    /* Add cloud extinction... */
    if (ctl->ncl > 0 && atm->cldz > 0) {
      double aux = exp(-0.5 * POW2((z - atm->clz) / atm->cldz));
      for (int id = 0; id < ctl->nd; id++) {
        int icl = locate_irr(ctl->clnu, ctl->ncl, ctl->nu[id]);
        los->k[los->np][id]
          += aux * LIN(ctl->clnu[icl], atm->clk[icl],
                       ctl->clnu[icl + 1], atm->clk[icl + 1], ctl->nu[id]);
      }
    }

    /* Increment and check number of LOS points... */
    if ((++los->np) > NLOS)
      ERRMSG("Too many LOS points!");

    /* Check stop flag... */
    if (stop) {

      /* Set surface temperature... */
      if (ctl->nsf > 0 && atm->sft > 0)
        t = atm->sft;
      los->sft = (stop == 2 ? t : -999);

      /* Set surface emissivity... */
      for (int id = 0; id < ctl->nd; id++) {
        los->sfeps[id] = 1.0;
        if (ctl->nsf > 0) {
          int isf = locate_irr(ctl->sfnu, ctl->nsf, ctl->nu[id]);
          los->sfeps[id] = LIN(ctl->sfnu[isf], atm->sfeps[isf],
                               ctl->sfnu[isf + 1], atm->sfeps[isf + 1],
                               ctl->nu[id]);
        }
      }

      /* Leave raytracer... */
      break;
    }

    /* Determine refractivity... */
    if (ctl->refrac && z <= zrefrac)
      n = 1 + refractivity(p, t);
    else
      n = 1;

```

```
    /* Construct new tangent vector (first term)... */
    for (int i = 0; i < 3; i++)
      ex1[i] = ex0[i] * n;

    /* Compute gradient of refractivity... */
    if (ctl->refrac && z <= zrefrac) {
      for (int i = 0; i < 3; i++)
        xh[i] = x[i] + 0.5 * ds * ex0[i];
      cart2geo(xh, &z, &lon, &lat);
      intpol_atm(ctl, atm, z, &p, &t, q, k);
      n = refractivity(p, t);
      for (int i = 0; i < 3; i++) {
        xh[i] += h;
        cart2geo(xh, &z, &lon, &lat);
        intpol_atm(ctl, atm, z, &p, &t, q, k);
        ng[i] = (refractivity(p, t) - n) / h;
        xh[i] -= h;
      }
    } else
      for (int i = 0; i < 3; i++)
        ng[i] = 0;

    /* Construct new tangent vector (second term)... */
    for (int i = 0; i < 3; i++)
      ex1[i] += ds * ng[i];

    /* Normalize new tangent vector... */
    norm = NORM(ex1);
    for (int i = 0; i < 3; i++)
      ex1[i] /= norm;

    /* Determine next point of LOS... */
    for (int i = 0; i < 3; i++)
      x[i] += 0.5 * ds * (ex0[i] + ex1[i]);

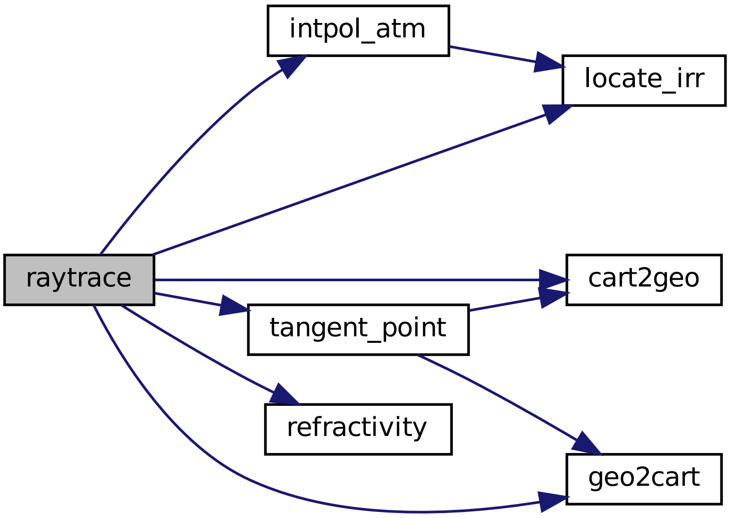
    /* Copy tangent vector... */
    for (int i = 0; i < 3; i++)
      ex0[i] = ex1[i];
  }

  /* Get tangent point (to be done before changing segment lengths!)... */
  tangent_point(los, &obs->tpz[ir], &obs->tplon[ir], &obs->tplat[ir]);

  /* Change segment lengths according to trapezoid rule... */
  for (int ip = los->np - 1; ip >= 1; ip--)
    los->ds[ip] = 0.5 * (los->ds[ip - 1] + los->ds[ip]);
  los->ds[0] *= 0.5;

  /* Compute column density... */
  for (int ip = 0; ip < los->np; ip++)
    for (int ig = 0; ig < ctl->ng; ig++)
      los->u[ip][ig] = 10 * los->q[ip][ig] * los->p[ip]
        / (KB * los->t[ip]) * los->ds[ip];
}
```

Here is the call graph for this function:



5.19.3.35 read_atm()

```
void read_atm (
    const char * dirname,
    const char * filename,
    ctl_t * ctl,
    atm_t * atm )
```

Read atmospheric data.

Definition at line 4331 of file jurassic.c.

```
                 {

  FILE *in;

  char file[LEN], line[LEN], *tok;

  /* Init... */
  atm->np = 0;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read atmospheric data: %s", file);

  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read line... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    TOK(line, tok, "%lg", atm->time[atm->np]);
    TOK(NULL, tok, "%lg", atm->z[atm->np]);
```

```
    TOK(NULL, tok, "%lg", atm->lon[atm->np]);
    TOK(NULL, tok, "%lg", atm->lat[atm->np]);
    TOK(NULL, tok, "%lg", atm->p[atm->np]);
    TOK(NULL, tok, "%lg", atm->t[atm->np]);
    for (int ig = 0; ig < ctl->ng; ig++)
      TOK(NULL, tok, "%lg", atm->q[ig][atm->np]);
    for (int iw = 0; iw < ctl->nw; iw++)
      TOK(NULL, tok, "%lg", atm->k[iw][atm->np]);
    if (ctl->ncl > 0 && atm->np == 0) {
      TOK(NULL, tok, "%lg", atm->clz);
      TOK(NULL, tok, "%lg", atm->cldz);
      for (int icl = 0; icl < ctl->ncl; icl++)
        TOK(NULL, tok, "%lg", atm->clk[icl]);
    }
    if (ctl->nsf > 0 && atm->np == 0) {
      TOK(NULL, tok, "%lg", atm->sfz);
      TOK(NULL, tok, "%lg", atm->sfp);
      TOK(NULL, tok, "%lg", atm->sft);
      for (int isf = 0; isf < ctl->nsf; isf++)
        TOK(NULL, tok, "%lg", atm->sfeps[isf]);
    }

    /* Increment data point counter... */
    if ((++atm->np) > NP)
      ERRMSG("Too many data points!");
  }

  /* Close file... */
  fclose(in);

  /* Check number of points... */
  if (atm->np < 1)
    ERRMSG("Could not read any data!");
}
```

5.19.3.36 read_ctl()

```
void read_ctl (
    int argc,
    char * argv[],
    ctl_t * ctl )
```

Read forward model control parameters.

Definition at line 4400 of file jurassic.c.

```
               {

  /* Write info... */
  LOG(1, "\nJuelich Rapid Spectral Simulation Code (JURASSIC)\n"
      "(executable: %s | version: %s | compiled: %s, %s)\n",
      argv[0], VERSION, __DATE__, __TIME__);

  /* Emitters... */
  ctl->ng = (int) scan_ctl(argc, argv, "NG", -1, "0", NULL);
  if (ctl->ng < 0 || ctl->ng > NG)
    ERRMSG("Set 0 <= NG <= MAX!");
  for (int ig = 0; ig < ctl->ng; ig++)
    scan_ctl(argc, argv, "EMITTER", ig, "", ctl->emitter[ig]);

  /* Radiance channels... */
  ctl->nd = (int) scan_ctl(argc, argv, "ND", -1, "0", NULL);
  if (ctl->nd < 0 || ctl->nd > ND)
    ERRMSG("Set 0 <= ND <= MAX!");
  for (int id = 0; id < ctl->nd; id++)
    ctl->nu[id] = scan_ctl(argc, argv, "NU", id, "", NULL);

  /* Spectral windows... */
  ctl->nw = (int) scan_ctl(argc, argv, "NW", -1, "1", NULL);
  if (ctl->nw < 0 || ctl->nw > NW)
    ERRMSG("Set 0 <= NW <= MAX!");
  for (int id = 0; id < ctl->nd; id++)
    ctl->window[id] = (int) scan_ctl(argc, argv, "WINDOW", id, "0", NULL);

  /* Cloud data... */
  ctl->ncl = (int) scan_ctl(argc, argv, "NCL", -1, "0", NULL);
  if (ctl->ncl < 0 || ctl->ncl > NCL)
    ERRMSG("Set 0 <= NCL <= MAX!");
  if (ctl->ncl == 1)
    ERRMSG("Set NCL > 1!");
  for (int icl = 0; icl < ctl->ncl; icl++)
```

```
    ctl->clnu[icl] = scan_ctl(argc, argv, "CLNU", icl, "", NULL);

  /* Surface data... */
  ctl->nsf = (int) scan_ctl(argc, argv, "NSF", -1, "0", NULL);
  if (ctl->nsf < 0 || ctl->nsf > NSF)
    ERRMSG("Set 0 <= NSF <= MAX!");
  if (ctl->nsf == 1)
    ERRMSG("Set NSF > 1!");
  for (int isf = 0; isf < ctl->nsf; isf++)
    ctl->sfnu[isf] = scan_ctl(argc, argv, "SFNU", isf, "", NULL);
  ctl->sftype = (int) scan_ctl(argc, argv, "SFTYPE", -1, "2", NULL);
  if (ctl->sftype < 0 || ctl->sftype > 3)
    ERRMSG("Set 0 <= SFTYPE <= 3!");
  ctl->sfsza = scan_ctl(argc, argv, "SFSZA", -1, "-999", NULL);

  /* Emissivity look-up tables... */
  scan_ctl(argc, argv, "TBLBASE", -1, "-", ctl->tblbase);
  ctl->tblfmt = (int) scan_ctl(argc, argv, "TBLFMT", -1, "1", NULL);

  /* Hydrostatic equilibrium... */
  ctl->hydz = scan_ctl(argc, argv, "HYDZ", -1, "-999", NULL);

  /* Continua... */
  ctl->ctm_co2 = (int) scan_ctl(argc, argv, "CTM_CO2", -1, "1", NULL);
  ctl->ctm_h2o = (int) scan_ctl(argc, argv, "CTM_H2O", -1, "1", NULL);
  ctl->ctm_n2 = (int) scan_ctl(argc, argv, "CTM_N2", -1, "1", NULL);
  ctl->ctm_o2 = (int) scan_ctl(argc, argv, "CTM_O2", -1, "1", NULL);

  /* Ray-tracing... */
  ctl->refrac = (int) scan_ctl(argc, argv, "REFRAC", -1, "1", NULL);
  ctl->rayds = scan_ctl(argc, argv, "RAYDS", -1, "10", NULL);
  ctl->raydz = scan_ctl(argc, argv, "RAYDZ", -1, "0.1", NULL);

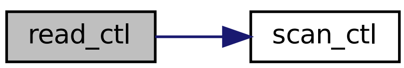
  /* Field of view... */
  scan_ctl(argc, argv, "FOV", -1, "-", ctl->fov);

  /* Retrieval interface... */
  ctl->retp_zmin = scan_ctl(argc, argv, "RETP_ZMIN", -1, "-999", NULL);
  ctl->retp_zmax = scan_ctl(argc, argv, "RETP_ZMAX", -1, "-999", NULL);
  ctl->rett_zmin = scan_ctl(argc, argv, "RETT_ZMIN", -1, "-999", NULL);
  ctl->rett_zmax = scan_ctl(argc, argv, "RETT_ZMAX", -1, "-999", NULL);
  for (int ig = 0; ig < ctl->ng; ig++) {
    ctl->retq_zmin[ig] = scan_ctl(argc, argv, "RETQ_ZMIN", ig, "-999", NULL);
    ctl->retq_zmax[ig] = scan_ctl(argc, argv, "RETQ_ZMAX", ig, "-999", NULL);
  }
  for (int iw = 0; iw < ctl->nw; iw++) {
    ctl->retk_zmin[iw] = scan_ctl(argc, argv, "RETK_ZMIN", iw, "-999", NULL);
    ctl->retk_zmax[iw] = scan_ctl(argc, argv, "RETK_ZMAX", iw, "-999", NULL);
  }
  ctl->ret_clz = (int) scan_ctl(argc, argv, "RET_CLZ", -1, "0", NULL);
  ctl->ret_cldz = (int) scan_ctl(argc, argv, "RET_CLDZ", -1, "0", NULL);
  ctl->ret_clk = (int) scan_ctl(argc, argv, "RET_CLK", -1, "0", NULL);
  ctl->ret_sfz = (int) scan_ctl(argc, argv, "RET_SFZ", -1, "0", NULL);
  ctl->ret_sfp = (int) scan_ctl(argc, argv, "RET_SFP", -1, "0", NULL);
  ctl->ret_sft = (int) scan_ctl(argc, argv, "RET_SFT", -1, "0", NULL);
  ctl->ret_sfeps = (int) scan_ctl(argc, argv, "RET_SFEPS", -1, "0", NULL);

  /* Output flags... */
  ctl->write_bbt = (int) scan_ctl(argc, argv, "WRITE_BBT", -1, "0", NULL);
  ctl->write_matrix =
    (int) scan_ctl(argc, argv, "WRITE_MATRIX", -1, "0", NULL);

  /* External forward models... */
  ctl->formod = (int) scan_ctl(argc, argv, "FORMOD", -1, "1", NULL);
  scan_ctl(argc, argv, "RFMBIN", -1, "-", ctl->rfmbin);
  scan_ctl(argc, argv, "RFMHIT", -1, "-", ctl->rfmhit);
  for (int ig = 0; ig < ctl->ng; ig++)
    scan_ctl(argc, argv, "RFMXSC", ig, "-", ctl->rfmxsc[ig]);
}
```

Here is the call graph for this function:



5.19.3.37 read_matrix() void read_matrix (

const char * *dirname*,
const char * *filename*,
gsl_matrix * *matrix*)

Read matrix.

Definition at line 4510 of file jurassic.c.

```
                        {

  FILE *in;

  char dum[LEN], file[LEN], line[LEN];

  double value;

  int i, j;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read matrix: %s", file);

  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read data... */
  gsl_matrix_set_zero(matrix);
  while (fgets(line, LEN, in))
    if (sscanf(line, "%d %s %s %s %s %s %d %s %s %s %s %s %lg",
               &i, dum, dum, dum, dum, dum,
               &j, dum, dum, dum, dum, dum, &value) == 13)
      gsl_matrix_set(matrix, (size_t) i, (size_t) j, value);

  /* Close file... */
  fclose(in);
}
```

5.19.3.38 read_obs() void read_obs (

const char * *dirname*,
const char * *filename*,
ctl_t * *ctl*,
obs_t * *obs*)

Read observation data.

Definition at line 4550 of file jurassic.c.

```
                {

  FILE *in;

  char file[LEN], line[LEN], *tok;

  /* Init... */
  obs->nr = 0;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Read observation data: %s", file);
```

```
  /* Open file... */
  if (!(in = fopen(file, "r")))
    ERRMSG("Cannot open file!");

  /* Read line... */
  while (fgets(line, LEN, in)) {

    /* Read data... */
    TOK(line, tok, "%lg", obs->time[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obsz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obslon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->obslat[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vpz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vplon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->vplat[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tpz[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tplon[obs->nr]);
    TOK(NULL, tok, "%lg", obs->tplat[obs->nr]);
    for (int id = 0; id < ctl->nd; id++)
      TOK(NULL, tok, "%lg", obs->rad[id][obs->nr]);
    for (int id = 0; id < ctl->nd; id++)
      TOK(NULL, tok, "%lg", obs->tau[id][obs->nr]);

    /* Increment counter... */
    if ((++obs->nr) > NR)
      ERRMSG("Too many rays!");
  }

  /* Close file... */
  fclose(in);

  /* Check number of points... */
  if (obs->nr < 1)
    ERRMSG("Could not read any data!");
}
```

5.19.3.39 read_obs_rfm()

```
double read_obs_rfm (
        const char * basename,
        double z,
        double * nu,
        double * f,
        int n )
```

Read observation data in RFM format.

Definition at line 4610 of file jurassic.c.

```
          {

  FILE *in;

  char filename[LEN];

  double filt, fsum = 0, nu2[NSHAPE], *nurfm, *rad, radsum = 0;

  int i, idx, ipts, npts;

  /* Allocate... */
  ALLOC(nurfm, double,
        RFMNPTS);
  ALLOC(rad, double,
        RFMNPTS);

  /* Search RFM spectrum... */
  sprintf(filename, "%s_%05d.asc", basename, (int) (z * 1000));
  if (!(in = fopen(filename, "r"))) {
    sprintf(filename, "%s_%05d.asc", basename, (int) (z * 1000) + 1);
    if (!(in = fopen(filename, "r")))
      ERRMSG("Cannot find RFM data file!");
  }
  fclose(in);

  /* Read RFM spectrum... */
  read_rfm_spec(filename, nurfm, rad, &npts);

  /* Set wavenumbers... */
  nu2[0] = nu[0];
```

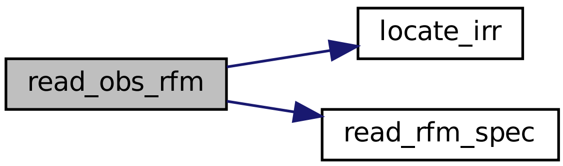
```
  nu2[n - 1] = nu[n - 1];
  for (i = 1; i < n - 1; i++)
    nu2[i] = LIN(0.0, nu2[0], n - 1.0, nu2[n - 1], i);

  /* Convolute... */
  for (ipts = 0; ipts < npts; ipts++)
    if (nurfm[ipts] >= nu2[0] && nurfm[ipts] <= nu2[n - 1]) {
      idx = locate_irr(nu2, n, nurfm[ipts]);
      filt = LIN(nu2[idx], f[idx], nu2[idx + 1], f[idx + 1], nurfm[ipts]);
      fsum += filt;
      radsum += filt * rad[ipts];
    }

  /* Free... */
  free(nurfm);
  free(rad);

  /* Return radiance... */
  return radsum / fsum;
}
```

Here is the call graph for this function:



5.19.3.40 read_rfm_spec()

```
void read_rfm_spec (
    const char * filename,
    double * nu,
    double * rad,
    int * npts )
```

Read RFM spectrum.

Definition at line 4668 of file jurassic.c.

```
                 {

  FILE *in;

  char line[RFMLINE], *tok;

  double dnu, nu0, nu1;

  int i, ipts = 0;

  /* Write info... */
  printf("Read RFM data: %s\n", filename);

  /* Open file... */
  if (!(in = fopen(filename, "r")))
    ERRMSG("Cannot open file!");

  /* Read header...... */
  for (i = 0; i < 4; i++)
    if (fgets(line, RFMLINE, in) == NULL)
      ERRMSG("Error while reading file header!");
  sscanf(line, "%d %lg %lg %lg", npts, &nu0, &dnu, &nu1);
  if (*npts > RFMNPTS)
```

```
    ERRMSG("Too many spectral grid points!");

  /* Read radiance data... */
  while (fgets(line, RFMLINE, in) && ipts < *npts - 1) {
    if ((tok = strtok(line, " \t\n")) != NULL)
      if (sscanf(tok, "%lg", &rad[ipts]) == 1)
        ipts++;
    while ((tok = strtok(NULL, " \t\n")) != NULL)
      if (sscanf(tok, "%lg", &rad[ipts]) == 1)
        ipts++;
  }
  if (ipts != *npts)
    ERRMSG("Error while reading RFM data!");

  /* Compute wavenumbers... */
  for (ipts = 0; ipts < *npts; ipts++)
    nu[ipts] = LIN(0.0, nu0, (double) (*npts - 1), nu1, (double) ipts);

  /* Close file... */
  fclose(in);
}
```

5.19.3.41 read_shape()

```
void read_shape (
        const char * filename,
        double * x,
        double * y,
        int * n )
```

Read shape function.

Definition at line 4719 of file jurassic.c.

```
                {

  FILE *in;

  char line[LEN];

  /* Write info... */
  LOG(1, "Read shape function: %s", filename);

  /* Open file... */
  if (!(in = fopen(filename, "r")))
    ERRMSG("Cannot open file!");

  /* Read data... */
  *n = 0;
  while (fgets(line, LEN, in))
    if (sscanf(line, "%lg %lg", &x[*n], &y[*n]) == 2)
      if ((++(*n)) > NSHAPE)
        ERRMSG("Too many data points!");

  /* Check number of points... */
  if (*n < 1)
    ERRMSG("Could not read any data!");

  /* Close file... */
  fclose(in);
}
```

5.19.3.42 read_tbl()

```
void read_tbl (
        ctl_t * ctl,
        tbl_t * tbl )
```

Read look-up table data.

Definition at line 4753 of file jurassic.c.

```
                     {

  FILE *in;
```

```
  char filename[2 * LEN], line[LEN];

  double eps, press, temp, u;

  /* Loop over trace gases and channels... */
  for (int id = 0; id < ctl->nd; id++)
    for (int ig = 0; ig < ctl->ng; ig++) {

      /* Initialize... */
      tbl->np[id][ig] = -1;
      double eps_old = -999;
      double press_old = -999;
      double temp_old = -999;
      double u_old = -999;

      /* Set filename... */
      sprintf(filename, "%s_%.4f_%s.%s", ctl->tblbase,
              ctl->nu[id], ctl->emitter[ig],
              ctl->tblfmt == 1 ? "tab" : "bin");

      /* Write info... */
      LOG(1, "Read emissivity table: %s", filename);

      /* Try to open file... */
      if (!(in = fopen(filename, "r"))) {
        WARN("Missing emissivity table: %s", filename);
        continue;
      }

      /* Read ASCII tables... */
      if (ctl->tblfmt == 1) {

        /* Read data... */
        while (fgets(line, LEN, in)) {

          /* Parse line... */
          if (sscanf(line, "%lg %lg %lg %lg", &press, &temp, &u, &eps) != 4)
            continue;

          /* Check ranges... */
          if (u < 0 || u > 1e30 || eps < 0 || eps > 1)
            continue;

          /* Determine pressure index... */
          if (press != press_old) {
            press_old = press;
            if ((++tbl->np[id][ig]) >= TBLNP)
              ERRMSG("Too many pressure levels!");
            tbl->nt[id][ig][tbl->np[id][ig]] = -1;
          }

          /* Determine temperature index... */
          if (temp != temp_old) {
            temp_old = temp;
            if ((++tbl->nt[id][ig][tbl->np[id][ig]]) >= TBLNT)
              ERRMSG("Too many temperatures!");
            tbl->nu[id][ig][tbl->np[id][ig]]
              [tbl->nt[id][ig][tbl->np[id][ig]]] = -1;
          }

          /* Determine column density index... */
          if ((eps > eps_old && u > u_old) || tbl->nu[id][ig][tbl->np[id][ig]]
              [tbl->nt[id][ig][tbl->np[id][ig]]] < 0) {
            eps_old = eps;
            u_old = u;
            if ((++tbl->nu[id][ig][tbl->np[id][ig]]
                 [tbl->nt[id][ig][tbl->np[id][ig]]]) >= TBLNU) {
              tbl->nu[id][ig][tbl->np[id][ig]]
                [tbl->nt[id][ig][tbl->np[id][ig]]]--;
              continue;
            }
          }

          /* Store data... */
          tbl->p[id][ig][tbl->np[id][ig]] = press;
          tbl->t[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
            = temp;
          tbl->u[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
            [tbl->nu[id][ig][tbl->np[id][ig]]
             [tbl->nt[id][ig][tbl->np[id][ig]]]] = (float) u;
          tbl->eps[id][ig][tbl->np[id][ig]][tbl->nt[id][ig][tbl->np[id][ig]]]
            [tbl->nu[id][ig][tbl->np[id][ig]]
             [tbl->nt[id][ig][tbl->np[id][ig]]]] = (float) eps;
        }

        /* Increment counters... */
```

```
      tbl->np[id][ig]++;
      for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
        tbl->nt[id][ig][ip]++;
        for (int it = 0; it < tbl->nt[id][ig][ip]; it++)
          tbl->nu[id][ig][ip][it]++;
      }
    }

    /* Read binary data... */
    else if (ctl->tblfmt == 2) {

      /* Read data... */
      FREAD(&tbl->np[id][ig], int,
            1,
            in);
      if (tbl->np[id][ig] > TBLNP)
        ERRMSG("Too many pressure levels!");
      FREAD(tbl->p[id][ig], double,
              (size_t) tbl->np[id][ig],
            in);
      for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
        FREAD(&tbl->nt[id][ig][ip], int,
              1,
              in);
        if (tbl->nt[id][ig][ip] > TBLNT)
          ERRMSG("Too many temperatures!");
        FREAD(tbl->t[id][ig][ip], double,
                (size_t) tbl->nt[id][ig][ip],
              in);
        for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
          FREAD(&tbl->nu[id][ig][ip][it], int,
                1,
                in);
          if (tbl->nu[id][ig][ip][it] > TBLNU)
            ERRMSG("Too many column densities!");
          FREAD(tbl->u[id][ig][ip][it], float,
                  (size_t) tbl->nu[id][ig][ip][it],
                in);
          FREAD(tbl->eps[id][ig][ip][it], float,
                  (size_t) tbl->nu[id][ig][ip][it],
                in);
        }
      }
    }

    /* Error message... */
    else
      ERRMSG("Unknown look-up table format!");

    /* Close file... */
    fclose(in);
  }
}
```

5.19.3.43 refractivity()

```
double refractivity (
    double p,
    double t )
```

Compute refractivity (return value is n - 1).

Definition at line 4901 of file jurassic.c.

```
                  {

  /* Refractivity of air at 4 to 15 micron... */
  return 7.753e-05 * p / t;
}
```

5.19.3.44 scan_ctl()

```
double scan_ctl (
    int argc,
    char * argv[],
    const char * varname,
```

```
int arridx,
const char * defvalue,
char * value )
```

Search control parameter file for variable entry.

Definition at line 4911 of file jurassic.c.

```
                  {

  FILE *in = NULL;

  char dummy[LEN], fullname1[LEN], fullname2[LEN], line[LEN],
    rvarname[LEN], rval[LEN];

  int contain = 0;

  /* Open file... */
  if (argv[1][0] != '-')
    if (!(in = fopen(argv[1], "r")))
      ERRMSG("Cannot open file!");

  /* Set full variable name... */
  if (arridx >= 0) {
    sprintf(fullname1, "%s[%d]", varname, arridx);
    sprintf(fullname2, "%s[*]", varname);
  } else {
    sprintf(fullname1, "%s", varname);
    sprintf(fullname2, "%s", varname);
  }

  /* Read data... */
  if (in != NULL)
    while (fgets(line, LEN, in))
      if (sscanf(line, "%s %s %s", rvarname, dummy, rval) == 3)
        if (strcasecmp(rvarname, fullname1) == 0 ||
            strcasecmp(rvarname, fullname2) == 0) {
          contain = 1;
          break;
        }
  for (int i = 1; i < argc - 1; i++)
    if (strcasecmp(argv[i], fullname1) == 0 ||
        strcasecmp(argv[i], fullname2) == 0) {
      sprintf(rval, "%s", argv[i + 1]);
      contain = 1;
      break;
    }

  /* Close file... */
  if (in != NULL)
    fclose(in);

  /* Check for missing variables... */
  if (!contain) {
    if (strlen(defvalue) > 0)
      sprintf(rval, "%s", defvalue);
    else
      ERRMSG("Missing variable %s!\n", fullname1);
  }

  /* Write info... */
  LOG(1, "%s = %s", fullname1, rval);

  /* Return values... */
  if (value != NULL)
    sprintf(value, "%s", rval);
  return atof(rval);
}
```

5.19.3.45 sza()

```
double sza (
double sec,
double lon,
double lat )
```

Calculate solar zenith angle.

Definition at line 4980 of file jurassic.c.

```
              {

  /* Number of days and fraction with respect to 2000-01-01T12:00Z... */
  double D = sec / 86400 - 0.5;

  /* Geocentric apparent ecliptic longitude [rad]... */
  double g = (357.529 + 0.98560028 * D) * M_PI / 180;
  double q = 280.459 + 0.98564736 * D;
  double L = (q + 1.915 * sin(g) + 0.020 * sin(2 * g)) * M_PI / 180;

  /* Mean obliquity of the ecliptic [rad]... */
  double e = (23.439 - 0.00000036 * D) * M_PI / 180;

  /* Declination [rad]... */
  double dec = asin(sin(e) * sin(L));

  /* Right ascension [rad]... */
  double ra = atan2(cos(e) * sin(L), cos(L));

  /* Greenwich Mean Sidereal Time [h]... */
  double GMST = 18.697374558 + 24.06570982441908 * D;

  /* Local Sidereal Time [h]... */
  double LST = GMST + lon / 15;

  /* Hour angle [rad]... */
  double h = LST / 12 * M_PI - ra;

  /* Convert latitude... */
  lat *= M_PI / 180;

  /* Return solar zenith angle [deg]... */
  return acos(sin(lat) * sin(dec) +
              cos(lat) * cos(dec) * cos(h)) * 180 / M_PI;
}
```

5.19.3.46 tangent_point()

```
void tangent_point (
        los_t * los,
        double * tpz,
        double * tplon,
        double * tplat )
```

Find tangent point of a given LOS.

Definition at line 5021 of file jurassic.c.

```
                 {

  double dummy, v[3], v0[3], v2[3];

  /* Find minimum altitude... */
  size_t ip = gsl_stats_min_index(los->z, 1, (size_t) los->np);

  /* Nadir or zenith... */
  if (ip <= 0 || ip >= (size_t) los->np - 1) {
    *tpz = los->z[los->np - 1];
    *tplon = los->lon[los->np - 1];
    *tplat = los->lat[los->np - 1];
  }

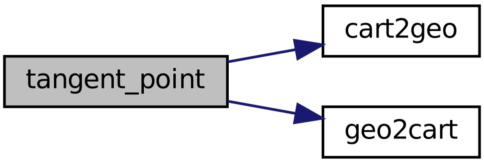
  /* Limb... */
  else {

    /* Determine interpolating polynomial y=a*x^2+b*x+c... */
    double yy0 = los->z[ip - 1];
    double yy1 = los->z[ip];
    double yy2 = los->z[ip + 1];
    double x1 = sqrt(POW2(los->ds[ip]) - POW2(yy1 - yy0));
    double x2 = x1 + sqrt(POW2(los->ds[ip + 1]) - POW2(yy2 - yy1));
    double a = 1 / (x1 - x2) * (-(yy0 - yy1) / x1 + (yy0 - yy2) / x2);
    double b = -(yy0 - yy1) / x1 - a * x1;
    double c = yy0;

    /* Get tangent point location... */
    double x = -b / (2 * a);
    *tpz = a * x * x + b * x + c;
    geo2cart(los->z[ip - 1], los->lon[ip - 1], los->lat[ip - 1], v0);
    geo2cart(los->z[ip + 1], los->lon[ip + 1], los->lat[ip + 1], v2);
```

```
    for (int i = 0; i < 3; i++)
      v[i] = LIN(0.0, v0[i], x2, v2[i], x);
    cart2geo(v, &dummy, tplon, tplat);
  }
}
```

Here is the call graph for this function:



5.19.3.47 time2jsec()

```
void time2jsec (
    int year,
    int mon,
    int day,
    int hour,
    int min,
    int sec,
    double remain,
    double * jsec )
```

Convert date to seconds.

Definition at line 5065 of file jurassic.c.

```
                  {

  struct tm t0, t1;

  t0.tm_year = 100;
  t0.tm_mon = 0;
  t0.tm_mday = 1;
  t0.tm_hour = 0;
  t0.tm_min = 0;
  t0.tm_sec = 0;

  t1.tm_year = year - 1900;
  t1.tm_mon = mon - 1;
  t1.tm_mday = day;
  t1.tm_hour = hour;
  t1.tm_min = min;
  t1.tm_sec = sec;

  *jsec = (double) timegm(&t1) - (double) timegm(&t0) + remain;
}
```

5.19.3.48 timer() void timer (

const char * *name*,
const char * *file*,
const char * *func*,
int *line*,
int *mode*)

Measure wall-clock time.

Definition at line 5096 of file jurassic.c.

```
              {

  static double w0[10];

  static int l0[10], nt;

  /* Start new timer... */
  if (mode == 1) {
    w0[nt] = omp_get_wtime();
    l0[nt] = line;
    if ((++nt) >= 10)
      ERRMSG("Too many timers!");
  }

  /* Write elapsed time... */
  else {

    /* Check timer index... */
    if (nt - 1 < 0)
      ERRMSG("Coding error!");

    /* Write elapsed time... */
    LOG(1, "Timer '%s' (%s, %s, l%d-%d): %.3f sec",
        name, file, func, l0[nt - 1], line, omp_get_wtime() - w0[nt - 1]);
  }

  /* Stop timer... */
  if (mode == 3)
    nt--;
}
```

5.19.3.49 write_atm() void write_atm (

const char * *dirname*,
const char * *filename*,
ctl_t * *ctl*,
atm_t * *atm*)

Write atmospheric data.

Definition at line 5134 of file jurassic.c.

```
                 {

  FILE *out;

  char file[LEN];

  int n = 6;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write atmospheric data: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
```

```
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = altitude [km]\n"
          "# $3 = longitude [deg]\n"
          "# $4 = latitude [deg]\n"
          "# $5 = pressure [hPa]\n" "# $6 = temperature [K]\n");
  for (int ig = 0; ig < ctl->ng; ig++)
    fprintf(out, "# $%d = %s volume mixing ratio [ppv]\n",
            ++n, ctl->emitter[ig]);
  for (int iw = 0; iw < ctl->nw; iw++)
    fprintf(out, "# $%d = extinction (window %d) [1/km]\n", ++n, iw);
  if (ctl->ncl > 0) {
    fprintf(out, "# $%d = cloud layer height [km]\n", ++n);
    fprintf(out, "# $%d = cloud layer depth [km]\n", ++n);
    for (int icl = 0; icl < ctl->ncl; icl++)
      fprintf(out, "# $%d = cloud layer extinction (%.4f cm^-1) [1/km]\n",
              ++n, ctl->clnu[icl]);
  }
  if (ctl->nsf > 0) {
    fprintf(out, "# $%d = surface layer height [km]\n", ++n);
    fprintf(out, "# $%d = surface layer pressure [hPa]\n", ++n);
    fprintf(out, "# $%d = surface layer temperature [K]\n", ++n);
    for (int isf = 0; isf < ctl->nsf; isf++)
      fprintf(out, "# $%d = surface layer emissivity (%.4f cm^-1)\n",
              ++n, ctl->sfnu[isf]);
  }

  /* Write data... */
  for (int ip = 0; ip < atm->np; ip++) {
    if (ip == 0 || atm->time[ip] != atm->time[ip - 1])
      fprintf(out, "\n");
    fprintf(out, "%.2f %g %g %g %g %g", atm->time[ip], atm->z[ip],
            atm->lon[ip], atm->lat[ip], atm->p[ip], atm->t[ip]);
    for (int ig = 0; ig < ctl->ng; ig++)
      fprintf(out, " %g", atm->q[ig][ip]);
    for (int iw = 0; iw < ctl->nw; iw++)
      fprintf(out, " %g", atm->k[iw][ip]);
    if (ctl->ncl > 0) {
      fprintf(out, " %g %g", atm->clz, atm->cldz);
      for (int icl = 0; icl < ctl->ncl; icl++)
        fprintf(out, " %g", atm->clk[icl]);
    }
    if (ctl->nsf > 0) {
      fprintf(out, " %g %g %g", atm->sfz, atm->sfp, atm->sft);
      for (int isf = 0; isf < ctl->nsf; isf++)
        fprintf(out, " %g", atm->sfeps[isf]);
    }
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);
}
```

5.19.3.50 write_atm_rfm()

```
void write_atm_rfm (
    const char * filename,
    ctl_t * ctl,
    atm_t * atm )
```

Write atmospheric data in RFM format.

Definition at line 5216 of file jurassic.c.

```
                    {

  FILE *out;

  int ig, ip;

  /* Write info... */
  printf("Write RFM data: %s\n", filename);

  /* Create file... */
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create file!");

  /* Write data... */
  fprintf(out, "%d\n", atm->np);
  fprintf(out, "*HGT [km]\n");
  for (ip = 0; ip < atm->np; ip++)
```

```
    fprintf(out, "%g\n", atm->z[ip]);
  fprintf(out, "*PRE [mb]\n");
  for (ip = 0; ip < atm->np; ip++)
    fprintf(out, "%g\n", atm->p[ip]);
  fprintf(out, "*TEM [K]\n");
  for (ip = 0; ip < atm->np; ip++)
    fprintf(out, "%g\n", atm->t[ip]);
  for (ig = 0; ig < ctl->ng; ig++) {
    fprintf(out, "*%s [ppmv]\n", ctl->emitter[ig]);
    for (ip = 0; ip < atm->np; ip++)
      fprintf(out, "%g\n", atm->q[ig][ip] * 1e6);
  }
  fprintf(out, "*END\n");

  /* Close file... */
  fclose(out);
}
```

5.19.3.51 write_matrix()

```
void write_matrix (
        const char * dirname,
        const char * filename,
        ctl_t * ctl,
        gsl_matrix * matrix,
        atm_t * atm,
        obs_t * obs,
        const char * rowspace,
        const char * colspace,
        const char * sort )
```

Write matrix.

Definition at line 5256 of file jurassic.c.

```
                         {

  FILE *out;

  char file[LEN], quantity[LEN];

  int *cida, *ciqa, *cipa, *cira, *rida, *riqa, *ripa, *rira;

  size_t i, j, nc, nr;

  /* Check output flag... */
  if (!ctl->write_matrix)
    return;

  /* Allocate... */
  ALLOC(cida, int,
        M);
  ALLOC(ciqa, int,
        N);
  ALLOC(cipa, int,
        N);
  ALLOC(cira, int,
        M);
  ALLOC(rida, int,
        M);
  ALLOC(riqa, int,
        N);
  ALLOC(ripa, int,
        N);
  ALLOC(rira, int,
        M);

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write matrix: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
```

```
    ERRMSG("Cannot create file!");

  /* Write header (row space)... */
  if (rowspace[0] == 'y') {

    fprintf(out,
            "# $1 = Row: index (measurement space)\n"
            "# $2 = Row: channel wavenumber [cm^-1]\n"
            "# $3 = Row: time (seconds since 2000-01-01T00:00Z)\n"
            "# $4 = Row: view point altitude [km]\n"
            "# $5 = Row: view point longitude [deg]\n"
            "# $6 = Row: view point latitude [deg]\n");

    /* Get number of rows... */
    nr = obs2y(ctl, obs, NULL, rida, rira);

  } else {

    fprintf(out,
            "# $1 = Row: index (state space)\n"
            "# $2 = Row: name of quantity\n"
            "# $3 = Row: time (seconds since 2000-01-01T00:00Z)\n"
            "# $4 = Row: altitude [km]\n"
            "# $5 = Row: longitude [deg]\n" "# $6 = Row: latitude [deg]\n");

    /* Get number of rows... */
    nr = atm2x(ctl, atm, NULL, riqa, ripa);
  }

  /* Write header (column space)... */
  if (colspace[0] == 'y') {

    fprintf(out,
            "# $7 = Col: index (measurement space)\n"
            "# $8 = Col: channel wavenumber [cm^-1]\n"
            "# $9 = Col: time (seconds since 2000-01-01T00:00Z)\n"
            "# $10 = Col: view point altitude [km]\n"
            "# $11 = Col: view point longitude [deg]\n"
            "# $12 = Col: view point latitude [deg]\n");

    /* Get number of columns... */
    nc = obs2y(ctl, obs, NULL, cida, cira);

  } else {

    fprintf(out,
            "# $7 = Col: index (state space)\n"
            "# $8 = Col: name of quantity\n"
            "# $9 = Col: time (seconds since 2000-01-01T00:00Z)\n"
            "# $10 = Col: altitude [km]\n"
            "# $11 = Col: longitude [deg]\n" "# $12 = Col: latitude [deg]\n");

    /* Get number of columns... */
    nc = atm2x(ctl, atm, NULL, ciqa, cipa);
  }

  /* Write header entry... */
  fprintf(out, "# $13 = Matrix element\n\n");

  /* Write matrix data... */
  i = j = 0;
  while (i < nr && j < nc) {

    /* Write info about the row... */
    if (rowspace[0] == 'y')
      fprintf(out, "%d %.4f %.2f %g %g %g",
              (int) i, ctl->nu[rida[i]],
              obs->time[rira[i]], obs->vpz[rira[i]],
              obs->vplon[rira[i]], obs->vplat[rira[i]]);
    else {
      idx2name(ctl, riqa[i], quantity);
      fprintf(out, "%d %s %.2f %g %g %g", (int) i, quantity,
              atm->time[ripa[i]], atm->z[ripa[i]],
              atm->lon[ripa[i]], atm->lat[ripa[i]]);
    }

    /* Write info about the column... */
    if (colspace[0] == 'y')
      fprintf(out, " %d %.4f %.2f %g %g %g",
              (int) j, ctl->nu[cida[j]],
              obs->time[cira[j]], obs->vpz[cira[j]],
              obs->vplon[cira[j]], obs->vplat[cira[j]]);
    else {
      idx2name(ctl, ciqa[j], quantity);
      fprintf(out, " %d %s %.2f %g %g %g", (int) j, quantity,
              atm->time[cipa[j]], atm->z[cipa[j]],
              atm->lon[cipa[j]], atm->lat[cipa[j]]);
```

```
    }

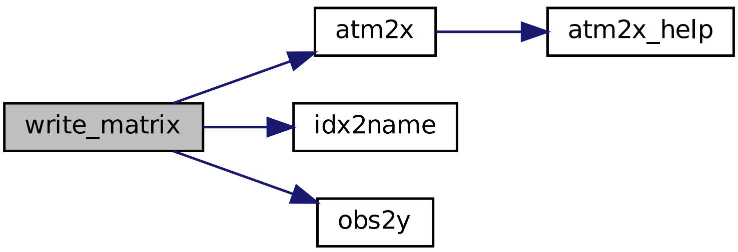
    /* Write matrix entry... */
    fprintf(out, " %g\n", gsl_matrix_get(matrix, i, j));

    /* Set matrix indices... */
    if (sort[0] == 'r') {
      j++;
      if (j >= nc) {
        j = 0;
        i++;
        fprintf(out, "\n");
      }
    } else {
      i++;
      if (i >= nr) {
        i = 0;
        j++;
        fprintf(out, "\n");
      }
    }
  }

  /* Close file... */
  fclose(out);

  /* Free... */
  free(cida);
  free(ciqa);
  free(cipa);
  free(cira);
  free(rida);
  free(riqa);
  free(ripa);
  free(rira);
}
```

Here is the call graph for this function:



5.19.3.52 write_obs() `void write_obs ( const char * dirname, const char * filename, ctl_t * ctl, obs_t * obs )`

Write observation data.

Definition at line 5434 of file jurassic.c.

```
                {

  FILE *out;
```

```

  char file[LEN];

  int n = 10;

  /* Set filename... */
  if (dirname != NULL)
    sprintf(file, "%s/%s", dirname, filename);
  else
    sprintf(file, "%s", filename);

  /* Write info... */
  LOG(1, "Write observation data: %s", file);

  /* Create file... */
  if (!(out = fopen(file, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n");
  for (int id = 0; id < ctl->nd; id++)
    fprintf(out, "# $%d = radiance (%.4f cm^-1) [W/(m^2 sr cm^-1)]\n",
            ++n, ctl->nu[id]);
  for (int id = 0; id < ctl->nd; id++)
    fprintf(out, "# $%d = transmittance (%.4f cm^-1) [-]\n", ++n,
            ctl->nu[id]);

  /* Write data... */
  for (int ir = 0; ir < obs->nr; ir++) {
    if (ir == 0 || obs->time[ir] != obs->time[ir - 1])
      fprintf(out, "\n");
    fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g", obs->time[ir],
            obs->obsz[ir], obs->obslon[ir], obs->obslat[ir],
            obs->vpz[ir], obs->vplon[ir], obs->vplat[ir],
            obs->tpz[ir], obs->tplon[ir], obs->tplat[ir]);
    for (int id = 0; id < ctl->nd; id++)
      fprintf(out, " %g", obs->rad[id][ir]);
    for (int id = 0; id < ctl->nd; id++)
      fprintf(out, " %g", obs->tau[id][ir]);
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);
}
```

5.19.3.53 write_shape()

```
void write_shape (
        const char * filename,
        double * x,
        double * y,
        int n )
```

Write shape function.

Definition at line 5499 of file jurassic.c.

```
         {

  FILE *out;

  /* Write info... */
  LOG(1, "Write shape function: %s", filename);

  /* Create file... */
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
```

```
  fprintf(out,
          "# $1 = shape function x-value [-]\n"
          "# $2 = shape function y-value [-]\n\n");

  /* Write data... */
  for (int i = 0; i < n; i++)
    fprintf(out, "%.10g %.10g\n", x[i], y[i]);

  /* Close file... */
  fclose(out);
}
```

5.19.3.54 write_tbl() void write_tbl (ctl_t * ctl, tbl_t * tbl)

Write look-up table data.

Definition at line 5529 of file jurassic.c.

```
                  {

  FILE *out;

  char filename[2 * LEN];

  /* Loop over emitters and detectors... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int id = 0; id < ctl->nd; id++) {

      /* Set filename... */
      sprintf(filename, "%s_%.4f_%s.%s", ctl->tblbase,
              ctl->nu[id], ctl->emitter[ig],
              ctl->tblfmt == 1 ? "tab" : "bin");

      /* Write info... */
      LOG(1, "Write emissivity table: %s", filename);

      /* Create file... */
      if (!(out = fopen(filename, "w")))
        ERRMSG("Cannot create file!");

      /* Write ASCII data... */
      if (ctl->tblfmt == 1) {

        /* Write header... */
        fprintf(out,
                "# $1 = pressure [hPa]\n"
                "# $2 = temperature [K]\n"
                "# $3 = column density [molecules/cm^2]\n"
                "# $4 = emissivity [-]\n");

        /* Save table file... */
        for (int ip = 0; ip < tbl->np[id][ig]; ip++)
          for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
            fprintf(out, "\n");
            for (int iu = 0; iu < tbl->nu[id][ig][ip][it]; iu++)
              fprintf(out, "%g %g %e %e\n",
                      tbl->p[id][ig][ip], tbl->t[id][ig][ip][it],
                      tbl->u[id][ig][ip][it][iu],
                      tbl->eps[id][ig][ip][it][iu]);
          }
      }

      /* Write binary data... */
      else if (ctl->tblfmt == 2) {
        FWRITE(&tbl->np[id][ig], int,
               1,
               out);
        FWRITE(tbl->p[id][ig], double,
                 (size_t) tbl->np[id][ig],
               out);
        for (int ip = 0; ip < tbl->np[id][ig]; ip++) {
          FWRITE(&tbl->nt[id][ig][ip], int,
                 1,
                 out);
          FWRITE(tbl->t[id][ig][ip], double,
                   (size_t) tbl->nt[id][ig][ip],
                 out);
```

```
        for (int it = 0; it < tbl->nt[id][ig][ip]; it++) {
          FWRITE(&tbl->nu[id][ig][ip][it], int,
                 1,
                 out);
          FWRITE(tbl->u[id][ig][ip][it], float,
                   (size_t) tbl->nu[id][ig][ip][it],
                 out);
          FWRITE(tbl->eps[id][ig][ip][it], float,
                   (size_t) tbl->nu[id][ig][ip][it],
                 out);
        }
      }
    }

    /* Error message... */
    else
      ERRMSG("Unknown look-up table format!");

    /* Close file... */
    fclose(out);
  }
}
```

5.19.3.55 x2atm()

```
void x2atm (
    ctl_t * ctl,
    gsl_vector * x,
    atm_t * atm )
```

Decompose parameter vector or state vector.

Definition at line 5615 of file jurassic.c.

```
                 {

  size_t n = 0;

  /* Get pressure... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->retp_zmin && atm->z[ip] <= ctl->retp_zmax)
      x2atm_help(&atm->p[ip], x, &n);

  /* Get temperature... */
  for (int ip = 0; ip < atm->np; ip++)
    if (atm->z[ip] >= ctl->rett_zmin && atm->z[ip] <= ctl->rett_zmax)
      x2atm_help(&atm->t[ip], x, &n);

  /* Get volume mixing ratio... */
  for (int ig = 0; ig < ctl->ng; ig++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retq_zmin[ig]
          && atm->z[ip] <= ctl->retq_zmax[ig])
        x2atm_help(&atm->q[ig][ip], x, &n);

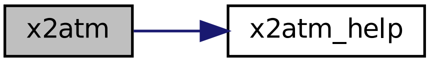
  /* Get extinction... */
  for (int iw = 0; iw < ctl->nw; iw++)
    for (int ip = 0; ip < atm->np; ip++)
      if (atm->z[ip] >= ctl->retk_zmin[iw]
          && atm->z[ip] <= ctl->retk_zmax[iw])
        x2atm_help(&atm->k[iw][ip], x, &n);

  /* Get cloud data... */
  if (ctl->ret_clz)
    x2atm_help(&atm->clz, x, &n);
  if (ctl->ret_cldz)
    x2atm_help(&atm->cldz, x, &n);
  if (ctl->ret_clk)
    for (int icl = 0; icl < ctl->ncl; icl++)
      x2atm_help(&atm->clk[icl], x, &n);

  /* Get surface data... */
  if (ctl->ret_sfz)
    x2atm_help(&atm->sfz, x, &n);
  if (ctl->ret_sfp)
    x2atm_help(&atm->sfp, x, &n);
  if (ctl->ret_sft)
    x2atm_help(&atm->sft, x, &n);
  if (ctl->ret_sfeps)
    for (int isf = 0; isf < ctl->nsf; isf++)
      x2atm_help(&atm->sfeps[isf], x, &n);
```

```
}
```

Here is the call graph for this function:



5.19.3.56 x2atm_help()

```
void x2atm_help (
    double * value,
    gsl_vector * x,
    size_t * n )
```

Get element from state vector.

Definition at line 5669 of file jurassic.c.

```
            {

  /* Get state vector element... */
  *value = gsl_vector_get(x, *n);
  (*n)++;
}
```

5.19.3.57 y2obs()

```
void y2obs (
    ctl_t * ctl,
    gsl_vector * y,
    obs_t * obs )
```

Decompose measurement vector.

Definition at line 5681 of file jurassic.c.

```
               {

  size_t m = 0;

  /* Decompose measurement vector... */
  for (int ir = 0; ir < obs->nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      if (gsl_finite(obs->rad[id][ir])) {
        obs->rad[id][ir] = gsl_vector_get(y, m);
        m++;
      }
}
```

5.20 jurassic.h

```
/*
  This file is part of JURASSIC.

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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

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  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#ifndef JURASSIC_H
#define JURASSIC_H

#include <gsl/gsl_math.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_linalg.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_statistics.h>
#include <math.h>
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <time.h>

/* ------------------------------------------------------------
   Macros...
   ------------------------------------------------------------ */

#define ALLOC(ptr, type, n)                              \
  if((ptr=malloc((size_t)(n)*sizeof(type)))==NULL)       \
    ERRMSG("Out of memory!");

#define DIST(a, b) sqrt(DIST2(a, b))

#define DIST2(a, b)                                                    \
  ((a[0]-b[0])*(a[0]-b[0])+(a[1]-b[1])*(a[1]-b[1])+(a[2]-b[2])*(a[2]-b[2]))

#define DOTP(a, b) (a[0]*b[0]+a[1]*b[1]+a[2]*b[2])

#define EXP(x0, y0, x1, y1, x)                                 \
  (((y0)>0 && (y1)>0)                                          \
   ? ((y0)*exp(log((y1)/(y0))/((x1)-(x0))*((x)-(x0))))         \
   : LIN(x0, y0, x1, y1, x))

#define FREAD(ptr, type, size, out) {                          \
    if(fread(ptr, sizeof(type), size, out)!=size)              \
      ERRMSG("Error while reading!");                          \
  }

#define FWRITE(ptr, type, size, out) {                         \
    if(fwrite(ptr, sizeof(type), size, out)!=size)             \
      ERRMSG("Error while writing!");                          \
  }

#define LIN(x0, y0, x1, y1, x)                   \
  ((y0)+((y1)-(y0))/((x1)-(x0))*((x)-(x0)))

#define NORM(a) sqrt(DOTP(a, a))

#define POW2(x) ((x)*(x))

#define POW3(x) ((x)*(x)*(x))

#define TIMER(name, mode)                                \
  {timer(name, __FILE__, __func__, __LINE__, mode);}

#define TOK(line, tok, format, var) {                    \
    if(((tok)=strtok((line), " \t"))) {                  \
      if(sscanf(tok, format, &(var))!=1) continue;       \
    } else ERRMSG("Error while reading!");               \
  }

/* ------------------------------------------------------------
   Log messages...
```

```
   ------------------------------------------------------------ */

#ifndef LOGLEV
#define LOGLEV 2
#endif

#define LOG(level, ...) {                                                   \
    if(level >= 2)                                                          \
      printf("  ");                                                         \
    if(level <= LOGLEV) {                                                   \
      printf(__VA_ARGS__);                                                  \
      printf("\n");                                                         \
    }                                                                       \
  }

#define WARN(...) {                                                         \
    printf("\nWarning (%s, %s, l%d): ", __FILE__, __func__, __LINE__);     \
    LOG(0, __VA_ARGS__);                                                    \
  }

#define ERRMSG(...) {                                                       \
    printf("\nError (%s, %s, l%d): ", __FILE__, __func__, __LINE__);       \
    LOG(0, __VA_ARGS__);                                                    \
    exit(EXIT_FAILURE);                                                     \
  }

#define PRINT(format, var)                                                  \
  printf("Print (%s, %s, l%d): %s= "format"\n",                            \
         __FILE__, __func__, __LINE__, #var, var);

/* ------------------------------------------------------------
   Constants...
   ------------------------------------------------------------ */

#define TMIN 100.

#define TMAX 400.

#define TSUN 5780.

#define C1 1.19104259e-8

#define C2 1.43877506

#define G0 9.80665

#define KB 1.3806504e-23

#define NA 6.02214199e23

#define H0 7.0

#define P0 1013.25

#define T0 273.15

#define RE 6367.421

#define RI 8.3144598

#define ME 5.976e24

/* ------------------------------------------------------------
   Dimensions...
   ------------------------------------------------------------ */

#ifndef NCL
#define NCL 8
#endif

#ifndef ND
#define ND 64
#endif

#ifndef NG
#define NG 8
#endif

#ifndef NP
#define NP 256
#endif

#ifndef NR
#define NR 256
#endif

#ifndef NSF
```

```
#define NSF 8
#endif

#ifndef NW
#define NW 4
#endif

#ifndef LEN
#define LEN 10000
#endif

#ifndef M
#define M (NR*ND)
#endif

#ifndef N
#define N ((2+NG+NW)*NP+NCL+NSF+5)
#endif

#ifndef NQ
#define NQ (7+NG+NW+NCL+NSF)
#endif

#ifndef NLOS
#define NLOS 4096
#endif

#ifndef NSHAPE
#define NSHAPE 10000
#endif

#ifndef NFOV
#define NFOV 5
#endif

#ifndef TBLNP
#define TBLNP 41
#endif

#ifndef TBLNT
#define TBLNT 30
#endif

#ifndef TBLNU
#define TBLNU 320
#endif

#ifndef TBLNS
#define TBLNS 1200
#endif

#ifndef RFMNPTS
#define RFMNPTS 10000000
#endif

#ifndef RFMLINE
#define RFMLINE 100000
#endif

/* ------------------------------------------------------------
   Quantity indices...
   ------------------------------------------------------------ */

#define IDXP 0

#define IDXT 1

#define IDXQ(ig) (2+ig)

#define IDXK(iw) (2+ctl->ng+iw)

#define IDXCLZ (2+ctl->ng+ctl->nw)

#define IDXCLDZ (3+ctl->ng+ctl->nw)

#define IDXCLK(icl) (4+ctl->ng+ctl->nw+icl)

#define IDXSFZ (4+ctl->ng+ctl->nw+ctl->ncl)

#define IDXSFP (5+ctl->ng+ctl->nw+ctl->ncl)

#define IDXSFT (6+ctl->ng+ctl->nw+ctl->ncl)

#define IDXSFEPS(isf) (7+ctl->ng+ctl->nw+ctl->ncl+isf)

/* ------------------------------------------------------------
   Structs...
```

```
   ------------------------------------------------------------ */

typedef struct {

  int np;

  double time[NP];

  double z[NP];

  double lon[NP];

  double lat[NP];

  double p[NP];

  double t[NP];

  double q[NG][NP];

  double k[NW][NP];

  double clz;

  double cldz;

  double clk[NCL];

  double sfz;

  double sfp;

  double sft;

  double sfeps[NSF];

} atm_t;

typedef struct {

  int ng;

  char emitter[NG][LEN];

  int nd;

  double nu[ND];

  int nw;

  int window[ND];

  int ncl;

  double clnu[NCL];

  int nsf;

  double sfnu[NSF];

  int sftype;

  double sfsza;

  char tblbase[LEN];

  int tblfmt;

  double hydz;

  int ctm_co2;

  int ctm_h2o;

  int ctm_n2;

  int ctm_o2;

  int refrac;

  double rayds;

  double raydz;

  char fov[LEN];

  double retp_zmin;
```

```
  double retp_zmax;
  double rett_zmin;
  double rett_zmax;
  double retq_zmin[NG];
  double retq_zmax[NG];
  double retk_zmin[NW];
  double retk_zmax[NW];
  int ret_clz;
  int ret_cldz;
  int ret_clk;
  int ret_sfz;
  int ret_sfp;
  int ret_sft;
  int ret_sfeps;
  int write_bbt;
  int write_matrix;
  int formod;
  char rfmbin[LEN];
  char rfmhit[LEN];
  char rfmxsc[NG][LEN];
} ctl_t;

typedef struct {
  int np;
  double z[NLOS];
  double lon[NLOS];
  double lat[NLOS];
  double p[NLOS];
  double t[NLOS];
  double q[NLOS][NG];
  double k[NLOS][ND];
  double sft;
  double sfeps[ND];
  double ds[NLOS];
  double u[NLOS][NG];
  double eps[NLOS][ND];
  double src[NLOS][ND];
} los_t;

typedef struct {
  int nr;
  double time[NR];
  double obsz[NR];
  double obslon[NR];
  double obslat[NR];
```

```
  double vpz[NR];

  double vplon[NR];

  double vplat[NR];

  double tpz[NR];

  double tplon[NR];

  double tplat[NR];

  double tau[ND][NR];

  double rad[ND][NR];

} obs_t;

typedef struct {

  int np[ND][NG];

  int nt[ND][NG][TBLNP];

  int nu[ND][NG][TBLNP][TBLNT];

  double p[ND][NG][TBLNP];

  double t[ND][NG][TBLNP][TBLNT];

  float u[ND][NG][TBLNP][TBLNT][TBLNU];

  float eps[ND][NG][TBLNP][TBLNT][TBLNU];

  double st[TBLNS];

  double sr[TBLNS][ND];

} tbl_t;

/* ------------------------------------------------------------
   Functions...
   ------------------------------------------------------------ */

size_t atm2x(
  ctl_t * ctl,
  atm_t * atm,
  gsl_vector * x,
  int *iqa,
  int *ipa);

void atm2x_help(
  double value,
  int value_iqa,
  int value_ip,
  gsl_vector * x,
  int *iqa,
  int *ipa,
  size_t *n);

double brightness(
  double rad,
  double nu);

void cart2geo(
  double *x,
  double *z,
  double *lon,
  double *lat);

void climatology(
  ctl_t * ctl,
  atm_t * atm_mean);

double ctmco2(
  double nu,
  double p,
  double t,
  double u);

double ctmh2o(
  double nu,
  double p,
  double t,
  double q,
  double u);

```

```
double ctmn2(
  double nu,
  double p,
  double t);

double ctmo2(
  double nu,
  double p,
  double t);

void copy_atm(
  ctl_t * ctl,
  atm_t * atm_dest,
  atm_t * atm_src,
  int init);

void copy_obs(
  ctl_t * ctl,
  obs_t * obs_dest,
  obs_t * obs_src,
  int init);

int find_emitter(
  ctl_t * ctl,
  const char *emitter);

void formod(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs);

void formod_continua(
  ctl_t * ctl,
  los_t * los,
  int ip,
  double *beta);

void formod_fov(
  ctl_t * ctl,
  obs_t * obs);

void formod_pencil(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs,
  int ir);

void formod_rfm(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs);

void formod_srcfunc(
  ctl_t * ctl,
  tbl_t * tbl,
  double t,
  double *src);

void geo2cart(
  double z,
  double lon,
  double lat,
  double *x);

void hydrostatic(
  ctl_t * ctl,
  atm_t * atm);

void idx2name(
  ctl_t * ctl,
  int idx,
  char *quantity);

void init_srcfunc(
  ctl_t * ctl,
  tbl_t * tbl);

void intpol_atm(
  ctl_t * ctl,
  atm_t * atm,
  double z,
  double *p,
  double *t,
  double *q,
  double *k);

void intpol_tbl(
```

```
  ctl_t * ctl,
  tbl_t * tbl,
  los_t * los,
  int ip,
  double tau_path[ND][NG],
  double tau_seg[ND]);

double intpol_tbl_eps(
  tbl_t * tbl,
  int ig,
  int id,
  int ip,
  int it,
  double u);

double intpol_tbl_u(
  tbl_t * tbl,
  int ig,
  int id,
  int ip,
  int it,
  double eps);

void jsec2time(
  double jsec,
  int *year,
  int *mon,
  int *day,
  int *hour,
  int *min,
  int *sec,
  double *remain);

void kernel(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs,
  gsl_matrix * k);

int locate_irr(
  double *xx,
  int n,
  double x);

int locate_reg(
  double *xx,
  int n,
  double x);

int locate_tbl(
  float *xx,
  int n,
  double x);

size_t obs2y(
  ctl_t * ctl,
  obs_t * obs,
  gsl_vector * y,
  int *ida,
  int *ira);

double planck(
  double t,
  double nu);

void raytrace(
  ctl_t * ctl,
  atm_t * atm,
  obs_t * obs,
  los_t * los,
  int ir);

void read_atm(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  atm_t * atm);

void read_ctl(
  int argc,
  char *argv[],
  ctl_t * ctl);

void read_matrix(
  const char *dirname,
  const char *filename,
  gsl_matrix * matrix);
```

```c

void read_obs(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  obs_t * obs);

double read_obs_rfm(
  const char *basename,
  double z,
  double *nu,
  double *f,
  int n);

void read_rfm_spec(
  const char *filename,
  double *nu,
  double *rad,
  int *npts);

void read_shape(
  const char *filename,
  double *x,
  double *y,
  int *n);

void read_tbl(
  ctl_t * ctl,
  tbl_t * tbl);

double refractivity(
  double p,
  double t);

double scan_ctl(
  int argc,
  char *argv[],
  const char *varname,
  int arridx,
  const char *defvalue,
  char *value);

double sza(
  double sec,
  double lon,
  double lat);

void tangent_point(
  los_t * los,
  double *tpz,
  double *tplon,
  double *tplat);

void time2jsec(
  int year,
  int mon,
  int day,
  int hour,
  int min,
  int sec,
  double remain,
  double *jsec);

void timer(
  const char *name,
  const char *file,
  const char *func,
  int line,
  int mode);

void write_atm(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  atm_t * atm);

void write_atm_rfm(
  const char *filename,
  ctl_t * ctl,
  atm_t * atm);

void write_matrix(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  gsl_matrix * matrix,
  atm_t * atm,
```

```
  obs_t * obs,
  const char *rowspace,
  const char *colspace,
  const char *sort);

void write_obs(
  const char *dirname,
  const char *filename,
  ctl_t * ctl,
  obs_t * obs);

void write_shape(
  const char *filename,
  double *x,
  double *y,
  int n);

void write_tbl(
  ctl_t * ctl,
  tbl_t * tbl);

void x2atm(
  ctl_t * ctl,
  gsl_vector * x,
  atm_t * atm);

void x2atm_help(
  double *value,
  gsl_vector * x,
  size_t *n);

void y2obs(
  ctl_t * ctl,
  gsl_vector * y,
  obs_t * obs);

#endif
```

5.21 kernel.c File Reference

Calculate kernel functions.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.21.1 Detailed Description

Calculate kernel functions.

Definition in file kernel.c.

5.21.2 Function Documentation

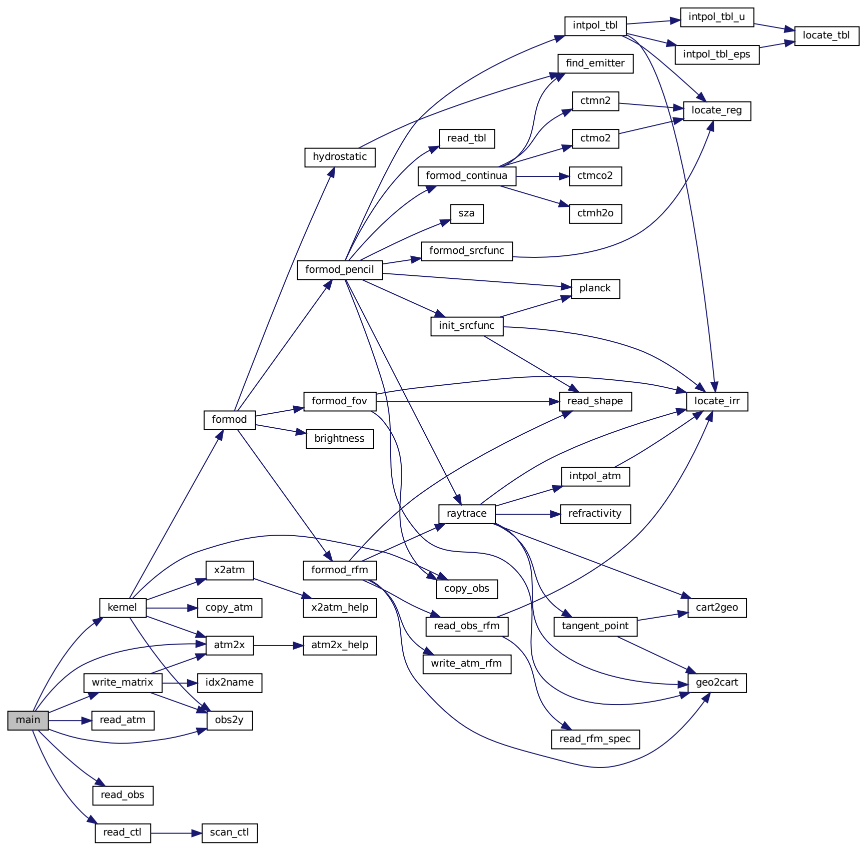
5.21.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file kernel.c.

```
                      {

  static atm_t atm;
  static ctl_t ctl;
  static obs_t obs;

  gsl_matrix *k;

  /* Check arguments... */
  if (argc < 5)
    ERRMSG("Give parameters: <ctl> <obs> <atm> <kernel>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Set flags... */
  ctl.write_matrix = 1;

  /* Read observation geometry... */
  read_obs(NULL, argv[2], &ctl, &obs);

  /* Read atmospheric data... */
  read_atm(NULL, argv[3], &ctl, &atm);

  /* Get sizes... */
  size_t n = atm2x(&ctl, &atm, NULL, NULL, NULL);
  size_t m = obs2y(&ctl, &obs, NULL, NULL, NULL);

  /* Check sizes... */
  if (n == 0)
    ERRMSG("No state vector elements!");
  if (m == 0)
    ERRMSG("No measurement vector elements!");

  /* Allocate... */
  k = gsl_matrix_alloc(m, n);

  /* Compute kernel matrix... */
  kernel(&ctl, &atm, &obs, k);

  /* Write matrix to file... */
  write_matrix(NULL, argv[4], &ctl, k, &atm, &obs, "y", "x", "r");

  /* Free... */
  gsl_matrix_free(k);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.22 kernel.c

```
/*
  This file is part of JURASSIC.

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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

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  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static atm_t atm;
  static ctl_t ctl;
  static obs_t obs;

  gsl_matrix *k;

  /* Check arguments... */
  if (argc < 5)
    ERRMSG("Give parameters: <ctl> <obs> <atm> <kernel>");
```

```
    /* Read control parameters... */
    read_ctl(argc, argv, &ctl);

    /* Set flags... */
    ctl.write_matrix = 1;

    /* Read observation geometry... */
    read_obs(NULL, argv[2], &ctl, &obs);

    /* Read atmospheric data... */
    read_atm(NULL, argv[3], &ctl, &atm);

    /* Get sizes... */
    size_t n = atm2x(&ctl, &atm, NULL, NULL, NULL);
    size_t m = obs2y(&ctl, &obs, NULL, NULL, NULL);

    /* Check sizes... */
    if (n == 0)
      ERRMSG("No state vector elements!");
    if (m == 0)
      ERRMSG("No measurement vector elements!");

    /* Allocate... */
    k = gsl_matrix_alloc(m, n);

    /* Compute kernel matrix... */
    kernel(&ctl, &atm, &obs, k);

    /* Write matrix to file... */
    write_matrix(NULL, argv[4], &ctl, k, &atm, &obs, "y", "x", "r");

    /* Free... */
    gsl_matrix_free(k);

    return EXIT_SUCCESS;
  }
```

5.23 limb.c File Reference

Create observation geometry for a limb sounder.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.23.1 Detailed Description

Create observation geometry for a limb sounder.

Definition in file limb.c.

5.23.2 Function Documentation

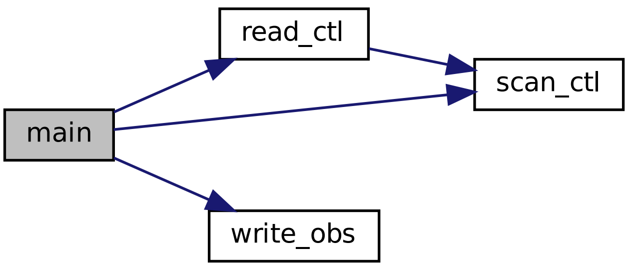
5.23.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file limb.c.

```
                {

  static ctl_t ctl;
  static obs_t obs;

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <obs>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  double obsz = scan_ctl(argc, argv, "OBSZ", -1, "780", NULL);
  double t0 = scan_ctl(argc, argv, "T0", -1, "0", NULL);
  double t1 = scan_ctl(argc, argv, "T1", -1, "0", NULL);
  double dt = scan_ctl(argc, argv, "DT", -1, "1", NULL);
  double z0 = scan_ctl(argc, argv, "Z0", -1, "3", NULL);
  double z1 = scan_ctl(argc, argv, "Z1", -1, "68", NULL);
  double dz = scan_ctl(argc, argv, "DZ", -1, "1", NULL);

  /* Create measurement geometry... */
  for (double t = t0; t <= t1; t += dt)
    for (double z = z0; z <= z1; z += dz) {
      obs.time[obs.nr] = t;
      obs.obsz[obs.nr] = obsz;
      obs.vpz[obs.nr] = z;
      obs.vplat[obs.nr] = 180 / M_PI * acos((RE + z) / (RE + obsz));
      if ((++obs.nr) >= NR)
        ERRMSG("Too many rays!");
    }

  /* Write observation data... */
  write_obs(NULL, argv[2], &ctl, &obs);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.24 limb.c

```
/*
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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

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  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
```

```
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static ctl_t ctl;
  static obs_t obs;

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <obs>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  double obsz = scan_ctl(argc, argv, "OBSZ", -1, "780", NULL);
  double t0 = scan_ctl(argc, argv, "T0", -1, "0", NULL);
  double t1 = scan_ctl(argc, argv, "T1", -1, "0", NULL);
  double dt = scan_ctl(argc, argv, "DT", -1, "1", NULL);
  double z0 = scan_ctl(argc, argv, "Z0", -1, "3", NULL);
  double z1 = scan_ctl(argc, argv, "Z1", -1, "68", NULL);
  double dz = scan_ctl(argc, argv, "DZ", -1, "1", NULL);

  /* Create measurement geometry... */
  for (double t = t0; t <= t1; t += dt)
    for (double z = z0; z <= z1; z += dz) {
      obs.time[obs.nr] = t;
      obs.obsz[obs.nr] = obsz;
      obs.vpz[obs.nr] = z;
      obs.vplat[obs.nr] = 180 / M_PI * acos((RE + z) / (RE + obsz));
      if ((++obs.nr) >= NR)
        ERRMSG("Too many rays!");
    }

  /* Write observation data... */
  write_obs(NULL, argv[2], &ctl, &obs);

  return EXIT_SUCCESS;
}
```

5.25 nadir.c File Reference

Create observation geometry for a nadir sounder.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.25.1 Detailed Description

Create observation geometry for a nadir sounder.

Definition in file nadir.c.

5.25.2 Function Documentation

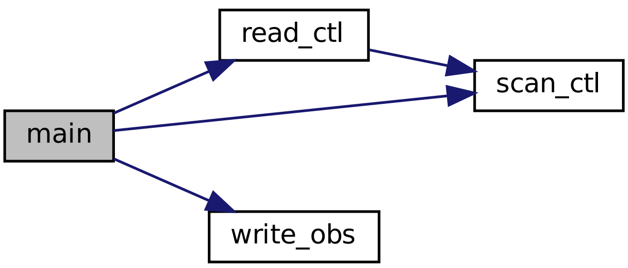
5.25.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file nadir.c.

```
                      {

  static ctl_t ctl;
  static obs_t obs;

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <obs>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  double t0 = scan_ctl(argc, argv, "T0", -1, "0", NULL);
  double t1 = scan_ctl(argc, argv, "T1", -1, "0", NULL);
  double dt = scan_ctl(argc, argv, "DT", -1, "1", NULL);
  double obsz = scan_ctl(argc, argv, "OBSZ", -1, "700", NULL);
  double lat0 = scan_ctl(argc, argv, "LAT0", -1, "-8.01", NULL);
  double lat1 = scan_ctl(argc, argv, "LAT1", -1, "8.01", NULL);
  double dlat = scan_ctl(argc, argv, "DLAT", -1, "0.18", NULL);

  /* Create measurement geometry... */
  for (double t = t0; t <= t1; t += dt)
    for (double lat = lat0; lat <= lat1; lat += dlat) {
      obs.time[obs.nr] = t;
      obs.obsz[obs.nr] = obsz;
      obs.vplat[obs.nr] = lat;
      if ((++obs.nr) >= NR)
        ERRMSG("Too many rays!");
    }

  /* Write observation data... */
  write_obs(NULL, argv[2], &ctl, &obs);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.26 nadir.c

```
/*
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  it under the terms of the GNU General Public License as published by
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  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.
```

```
  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static ctl_t ctl;
  static obs_t obs;

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <obs>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  double t0 = scan_ctl(argc, argv, "T0", -1, "0", NULL);
  double t1 = scan_ctl(argc, argv, "T1", -1, "0", NULL);
  double dt = scan_ctl(argc, argv, "DT", -1, "1", NULL);
  double obsz = scan_ctl(argc, argv, "OBSZ", -1, "700", NULL);
  double lat0 = scan_ctl(argc, argv, "LAT0", -1, "-8.01", NULL);
  double lat1 = scan_ctl(argc, argv, "LAT1", -1, "8.01", NULL);
  double dlat = scan_ctl(argc, argv, "DLAT", -1, "0.18", NULL);

  /* Create measurement geometry... */
  for (double t = t0; t <= t1; t += dt)
    for (double lat = lat0; lat <= lat1; lat += dlat) {
      obs.time[obs.nr] = t;
      obs.obsz[obs.nr] = obsz;
      obs.vplat[obs.nr] = lat;
      if ((++obs.nr) >= NR)
        ERRMSG("Too many rays!");
    }

  /* Write observation data... */
  write_obs(NULL, argv[2], &ctl, &obs);

  return EXIT_SUCCESS;
}
```

5.27 obs2spec.c File Reference

Converter for spectra.

```
#include <omp.h>
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.27.1 Detailed Description

Converter for spectra.

Definition in file obs2spec.c.

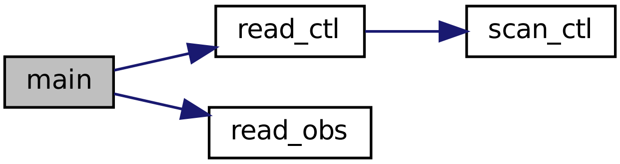
5.27.2 Function Documentation

5.27.2.1 main() int main (int argc, char * argv[])

Definition at line 32 of file obs2spec.c.

```
{

  static ctl_t ctl;

  obs_t *obs;

  FILE *out;

  /* Check arguments... */
  if (argc < 4)
    ERRMSG("Give parameters: <ctl> <obs> <spec.tab>");

  /* Allocate... */
  ALLOC(obs, obs_t, 1);

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Read observation geometry... */
  read_obs(".", argv[2], &ctl, obs);

  /* Write info... */
  LOG(1, "Write spectra: %s", argv[3]);

  /* Create file... */
  if (!(out = fopen(argv[3], "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n"
          "# $11 = channel frequency [cm^-1]\n"
          "# $12 = channel radiance [W/(m^2 sr cm^-1)]\n"
          "# $13 = channel transmittance [1]\n");

  /* Write data... */
  for (int ir = 0; ir < obs->nr; ir++) {
    fprintf(out, "\n");
    for (int id = 0; id < ctl.nd; id++)
      fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g %.4f %g %g\n",
              obs->time[ir], obs->obsz[ir], obs->obslon[ir], obs->obslat[ir],
              obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], obs->tpz[ir],
              obs->tplon[ir], obs->tplat[ir], ctl.nu[id], obs->rad[id][ir],
              obs->tau[id][ir]);
  }

  /* Close file... */
  fclose(out);

  /* Free... */
  free(obs);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.28 obs2spec.c

```c
/*
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  it under the terms of the GNU General Public License as published by
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  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include <omp.h>
#include "jurassic.h"

/* ------------------------------------------------------------
   Main...
   ------------------------------------------------------------ */

int main(
  int argc,
  char *argv[]) {

  static ctl_t ctl;

  obs_t *obs;

  FILE *out;

  /* Check arguments... */
  if (argc < 4)
    ERRMSG("Give parameters: <ctl> <obs> <spec.tab>");

  /* Allocate... */
  ALLOC(obs, obs_t, 1);

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Read observation geometry... */
  read_obs(".", argv[2], &ctl, obs);

  /* Write info... */
  LOG(1, "Write spectra: %s", argv[3]);

  /* Create file... */
  if (!(out = fopen(argv[3], "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
```

```
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n"
          "# $11 = channel frequency [cm^-1]\n"
          "# $12 = channel radiance [W/(m^2 sr cm^-1)]\n"
          "# $13 = channel transmittance [1]\n");

  /* Write data... */
  for (int ir = 0; ir < obs->nr; ir++) {
    fprintf(out, "\n");
    for (int id = 0; id < ctl.nd; id++)
      fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g %.4f %g %g\n",
              obs->time[ir], obs->obsz[ir], obs->obslon[ir], obs->obslat[ir],
              obs->vpz[ir], obs->vplon[ir], obs->vplat[ir], obs->tpz[ir],
              obs->tplon[ir], obs->tplat[ir], ctl.nu[id], obs->rad[id][ir],
              obs->tau[id][ir]);
  }

  /* Close file... */
  fclose(out);

  /* Free... */
  free(obs);

  return EXIT_SUCCESS;
}
```

5.29 planck.c File Reference

Convert brightness temperature to radiance.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.29.1 Detailed Description

Convert brightness temperature to radiance.

Definition in file planck.c.

5.29.2 Function Documentation

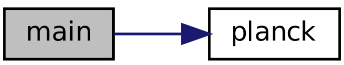
5.29.2.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 27 of file planck.c.

```
                  {

  /* Check arguments... */
  if (argc != 3 && argc != 7)
    ERRMSG
      ("Give parameters: [ <t> <nu> |  <t0> <t1> <dt> <nu0> <nu1> <dnu> ]");

  /* Calculate single value... */
  if (argc == 3) {

    /* Read arguments... */
    double t = atof(argv[1]);
    double nu = atof(argv[2]);

    /* Compute Planck function... */
    printf("%.10g\n", planck(t, nu));
  }

  /* Calculate table... */
  else if (argc == 7) {

    /* Read arguments... */
    double t0 = atof(argv[1]);
    double t1 = atof(argv[2]);
    double dt = atof(argv[3]);
    double nu0 = atof(argv[4]);
    double nu1 = atof(argv[5]);
    double dnu = atof(argv[6]);

    /* Write header... */
    printf("# $1 = brightness temperature [K]\n"
           "# $2 = wavenumber [cm^-1]\n"
           "# $3 = radiance [W/(m^2 sr cm^-1)]\n");

    /* Compute Planck function... */
    for (double t = t0; t <= t1; t += dt) {
      printf("\n");
      for (double nu = nu0; nu <= nu1; nu += dnu)
        printf("%.10g %.4f %.10g\n", t, nu, planck(t, nu));
    }
  }

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.30 planck.c

```
/*
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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

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  but WITHOUT ANY WARRANTY; without even the implied warranty of
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  GNU General Public License for more details.
```

```
  You should have received a copy of the GNU General Public License
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  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  /* Check arguments... */
  if (argc != 3 && argc != 7)
    ERRMSG
      ("Give parameters: [ <t> <nu> |  <t0> <t1> <dt> <nu0> <nu1> <dnu> ]");

  /* Calculate single value... */
  if (argc == 3) {

    /* Read arguments... */
    double t = atof(argv[1]);
    double nu = atof(argv[2]);

    /* Compute Planck function... */
    printf("%.10g\n", planck(t, nu));
  }

  /* Calculate table... */
  else if (argc == 7) {

    /* Read arguments... */
    double t0 = atof(argv[1]);
    double t1 = atof(argv[2]);
    double dt = atof(argv[3]);
    double nu0 = atof(argv[4]);
    double nu1 = atof(argv[5]);
    double dnu = atof(argv[6]);

    /* Write header... */
    printf("# $1 = brightness temperature [K]\n"
           "# $2 = wavenumber [cm^-1]\n"
           "# $3 = radiance [W/(m^2 sr cm^-1)]\n");

    /* Compute Planck function... */
    for (double t = t0; t <= t1; t += dt) {
      printf("\n");
      for (double nu = nu0; nu <= nu1; nu += dnu)
        printf("%.10g %.4f %.10g\n", t, nu, planck(t, nu));
    }
  }

  return EXIT_SUCCESS;
}
```

5.31 raytrace.c File Reference

Determine atmospheric ray paths.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char *argv[ ])

5.31.1 Detailed Description

Determine atmospheric ray paths.

Definition in file raytrace.c.

5.31.2 Function Documentation

5.31.2.1 main()

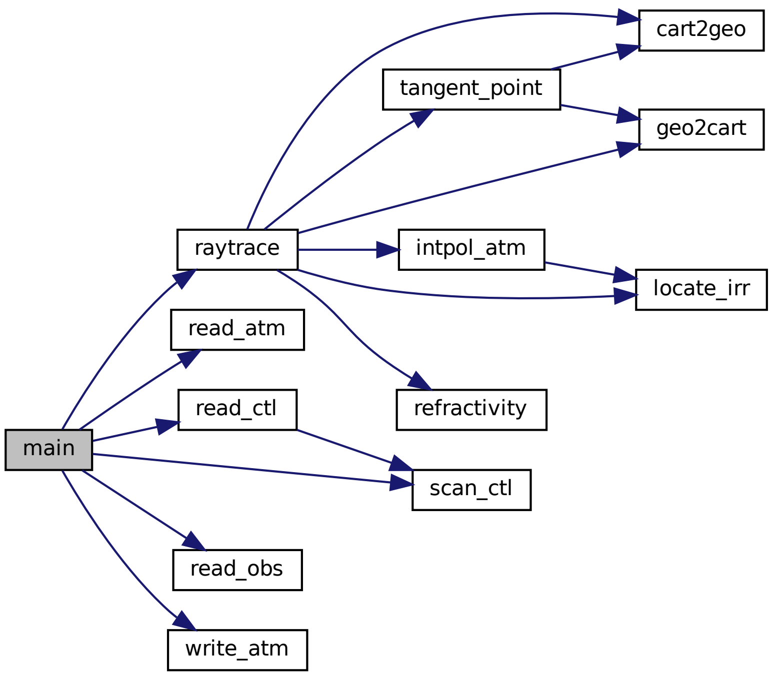
```
int main (
        int argc,
        char * argv[ ] )
```

Definition at line 27 of file raytrace.c.

```
                   {

  static atm_t atm, atm2;
  static ctl_t ctl;
  static los_t los;
  static obs_t obs;

  FILE *out;

  char filename[LEN], losbase[LEN];

  double u[NG];

  /* Check arguments... */
  if (argc < 4)
    ERRMSG("Give parameters: <ctl> <obs> <atm>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Get basenames... */
  scan_ctl(argc, argv, "LOSBASE", -1, "los", losbase);

  /* Read observation geometry... */
  read_obs(NULL, argv[2], &ctl, &obs);

  /* Read atmospheric data... */
  read_atm(NULL, argv[3], &ctl, &atm);

  /* Write info... */
  LOG(1, "Write raytrace data: raytrace.tab");

  /* Create file... */
  if (!(out = fopen("raytrace.tab", "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n"
          "# $11 = ray path index\n" "# $12 = ray path length [km]\n");
  for (int ig = 0; ig < ctl.ng; ig++)
    fprintf(out, "# $%d = %s column density [molec/cm^2]\n",
            13 + ig, ctl.emitter[ig]);
  fprintf(out, "\n");

  /* Loop over rays... */
  for (int ir = 0; ir < obs.nr; ir++) {

    /* Raytracing... */
    raytrace(&ctl, &atm, &obs, &los, ir);

    /* Copy data... */
    atm2.np = los.np;
    for (int ip = 0; ip < los.np; ip++) {
      atm2.time[ip] = obs.time[ir];
      atm2.z[ip] = los.z[ip];
      atm2.lon[ip] = los.lon[ip];
      atm2.lat[ip] = los.lat[ip];
      atm2.p[ip] = los.p[ip];
      atm2.t[ip] = los.t[ip];
      for (int ig = 0; ig < ctl.ng; ig++)
        atm2.q[ig][ip] = los.q[ip][ig];
      for (int iw = 0; iw < ctl.nw; iw++)
```

```
        atm2.k[iw][ip] = GSL_NAN;
    }

    /* Save data... */
    sprintf(filename, "los.%d", ir);
    write_atm(NULL, filename, &ctl, &atm2);

    /* Get column densities... */
    double s = 0;
    for (int ig = 0; ig < ctl.ng; ig++)
      u[ig] = 0;
    for (int ip = 0; ip < los.np; ip++) {
      s += los.ds[ip];
      for (int ig = 0; ig < ctl.ng; ig++)
        u[ig] += los.u[ip][ig];
    }

    /* Write summary data... */
    fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g %d %g",
            obs.time[ir], obs.obsz[ir], obs.obslon[ir], obs.obslat[ir],
            obs.vpz[ir], obs.vplon[ir], obs.vplat[ir],
            obs.tpz[ir], obs.tplon[ir], obs.tplat[ir], ir, s);
    for (int ig = 0; ig < ctl.ng; ig++)
      fprintf(out, " %g", u[ig]);
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.32 raytrace.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
```

```
  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  static atm_t atm, atm2;
  static ctl_t ctl;
  static los_t los;
  static obs_t obs;

  FILE *out;

  char filename[LEN], losbase[LEN];

  double u[NG];

  /* Check arguments... */
  if (argc < 4)
    ERRMSG("Give parameters: <ctl> <obs> <atm>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Get basenames... */
  scan_ctl(argc, argv, "LOSBASE", -1, "los", losbase);

  /* Read observation geometry... */
  read_obs(NULL, argv[2], &ctl, &obs);

  /* Read atmospheric data... */
  read_atm(NULL, argv[3], &ctl, &atm);

  /* Write info... */
  LOG(1, "Write raytrace data: raytrace.tab");

  /* Create file... */
  if (!(out = fopen("raytrace.tab", "w")))
    ERRMSG("Cannot create file!");

  /* Write header... */
  fprintf(out,
          "# $1 = time (seconds since 2000-01-01T00:00Z)\n"
          "# $2 = observer altitude [km]\n"
          "# $3 = observer longitude [deg]\n"
          "# $4 = observer latitude [deg]\n"
          "# $5 = view point altitude [km]\n"
          "# $6 = view point longitude [deg]\n"
          "# $7 = view point latitude [deg]\n"
          "# $8 = tangent point altitude [km]\n"
          "# $9 = tangent point longitude [deg]\n"
          "# $10 = tangent point latitude [deg]\n"
          "# $11 = ray path index\n" "# $12 = ray path length [km]\n");
  for (int ig = 0; ig < ctl.ng; ig++)
    fprintf(out, "# $%d = %s column density [molec/cm^2]\n",
            13 + ig, ctl.emitter[ig]);
  fprintf(out, "\n");

  /* Loop over rays... */
  for (int ir = 0; ir < obs.nr; ir++) {

    /* Raytracing... */
    raytrace(&ctl, &atm, &obs, &los, ir);

    /* Copy data... */
    atm2.np = los.np;
    for (int ip = 0; ip < los.np; ip++) {
      atm2.time[ip] = obs.time[ir];
      atm2.z[ip] = los.z[ip];
      atm2.lon[ip] = los.lon[ip];
      atm2.lat[ip] = los.lat[ip];
      atm2.p[ip] = los.p[ip];
```

```
      atm2.t[ip] = los.t[ip];
      for (int ig = 0; ig < ctl.ng; ig++)
        atm2.q[ig][ip] = los.q[ip][ig];
      for (int iw = 0; iw < ctl.nw; iw++)
        atm2.k[iw][ip] = GSL_NAN;
    }

    /* Save data... */
    sprintf(filename, "los.%d", ir);
    write_atm(NULL, filename, &ctl, &atm2);

    /* Get column densities... */
    double s = 0;
    for (int ig = 0; ig < ctl.ng; ig++)
      u[ig] = 0;
    for (int ip = 0; ip < los.np; ip++) {
      s += los.ds[ip];
      for (int ig = 0; ig < ctl.ng; ig++)
        u[ig] += los.u[ip][ig];
    }

    /* Write summary data... */
    fprintf(out, "%.2f %g %g %g %g %g %g %g %g %g %d %g",
            obs.time[ir], obs.obsz[ir], obs.obslon[ir], obs.obslat[ir],
            obs.vpz[ir], obs.vplon[ir], obs.vplat[ir],
            obs.tpz[ir], obs.tplon[ir], obs.tplat[ir], ir, s);
    for (int ig = 0; ig < ctl.ng; ig++)
      fprintf(out, " %g", u[ig]);
    fprintf(out, "\n");
  }

  /* Close file... */
  fclose(out);

  return EXIT_SUCCESS;
}
```

5.33 retrieval.c File Reference

JURASSIC retrieval processor.

```
#include "jurassic.h"
```

Data Structures

- struct ret_t

  Retrieval control parameters.

Functions

- void analyze_avk (ret_t *ret, ctl_t *ctl, atm_t *atm, int *iqa, int *ipa, gsl_matrix *avk)

  Compute information content and resolution.
- void analyze_avk_quantity (gsl_matrix *avk, int iq, int *ipa, size_t *n0, size_t *n1, double *cont, double *res)

  Analyze averaging kernels for individual retrieval target.
- double cost_function (gsl_vector *dx, gsl_vector *dy, gsl_matrix *s_a_inv, gsl_vector *sig_eps_inv)

  Compute cost function.
- void matrix_invert (gsl_matrix *a)

  Invert symmetric matrix.
- void matrix_product (gsl_matrix *a, gsl_vector *b, int transpose, gsl_matrix *c)

  Compute matrix product A^TBA or ABA^T for diagonal matrix B.
- void optimal_estimation (ret_t *ret, ctl_t *ctl, obs_t *obs_meas, obs_t *obs_i, atm_t *atm_apr, atm_t *atm_i)

  Carry out optimal estimation retrieval.
- void read_ret (int argc, char *argv[], ctl_t *ctl, ret_t *ret)

Read retrieval control parameters.

- void set_cov_apr (ret_t *ret, ctl_t *ctl, atm_t *atm, int *iqa, int *ipa, gsl_matrix *s_a)

  Set a priori covariance.

- void set_cov_meas (ret_t *ret, ctl_t *ctl, obs_t *obs, gsl_vector *sig_noise, gsl_vector *sig_formod, gsl_↩ vector *sig_eps_inv)

  Set measurement errors.

- void write_stddev (const char *quantity, ret_t *ret, ctl_t *ctl, atm_t *atm, gsl_matrix *s)

  Write retrieval error to file.

- int main (int argc, char *argv[ ])

5.33.1 Detailed Description

JURASSIC retrieval processor.

Definition in file retrieval.c.

5.33.2 Function Documentation

5.33.2.1 analyze_avk()

```
void analyze_avk (
        ret_t * ret,
        ctl_t * ctl,
        atm_t * atm,
        int * iqa,
        int * ipa,
        gsl_matrix * avk )
```

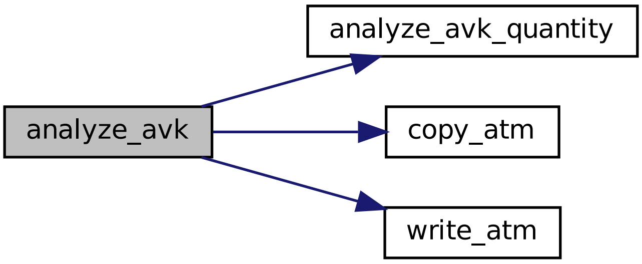
Compute information content and resolution.

Definition at line 257 of file retrieval.c.

```
00263                          {
00264 
00265   static atm_t atm_cont, atm_res;
00266 
00267   int icl, ig, iq, isf, iw;
00268 
00269   size_t i, n, n0[NQ], n1[NQ];
00270 
00271   /* Get sizes... */
00272   n = avk->size1;
00273 
00274   /* Find sub-matrices for different quantities... */
00275   for (iq = 0; iq < NQ; iq++) {
00276     n0[iq] = N;
00277     for (i = 0; i < n; i++) {
00278       if (iqa[i] == iq && n0[iq] == N)
00279         n0[iq] = i;
00280       if (iqa[i] == iq)
00281         n1[iq] = i - n0[iq] + 1;
00282     }
00283   }
00284 
00285   /* Initialize... */
00286   copy_atm(ctl, &atm_cont, atm, 1);
00287   copy_atm(ctl, &atm_res, atm, 1);
00288 
00289   /* Analyze quantities... */
00290   analyze_avk_quantity(avk, IDXP, ipa, n0, n1, atm_cont.p, atm_res.p);
00291   analyze_avk_quantity(avk, IDXT, ipa, n0, n1, atm_cont.t, atm_res.t);
00292   for (ig = 0; ig < ctl->ng; ig++)
00293     analyze_avk_quantity(avk, IDXQ(ig), ipa, n0, n1,
00294                          atm_cont.q[ig], atm_res.q[ig]);
00295   for (iw = 0; iw < ctl->nw; iw++)
```

```
    analyze_avk_quantity(avk, IDXK(iw), ipa, n0, n1,
                         atm_cont.k[iw], atm_res.k[iw]);
  analyze_avk_quantity(avk, IDXCLZ, ipa, n0, n1, &atm_cont.clz, &atm_res.clz);
  analyze_avk_quantity(avk, IDXCLDZ, ipa, n0, n1, &atm_cont.cldz,
                       &atm_res.cldz);
  for (icl = 0; icl < ctl->ncl; icl++)
    analyze_avk_quantity(avk, IDXCLK(icl), ipa, n0, n1,
                         &atm_cont.clk[icl], &atm_res.clk[icl]);
  analyze_avk_quantity(avk, IDXSFZ, ipa, n0, n1, &atm_cont.sfz, &atm_res.sfz);
  analyze_avk_quantity(avk, IDXSFP, ipa, n0, n1, &atm_cont.sfp, &atm_res.sfp);
  analyze_avk_quantity(avk, IDXSFT, ipa, n0, n1, &atm_cont.sft, &atm_res.sft);
  for (isf = 0; isf < ctl->nsf; isf++)
    analyze_avk_quantity(avk, IDXSFEPS(isf), ipa, n0, n1,
                         &atm_cont.sfeps[isf], &atm_res.sfeps[isf]);

  /* Write results to disk... */
  write_atm(ret->dir, "atm_cont.tab", ctl, &atm_cont);
  write_atm(ret->dir, "atm_res.tab", ctl, &atm_res);
}
```

Here is the call graph for this function:



5.33.2.2 analyze_avk_quantity()

```
void analyze_avk_quantity (
    gsl_matrix * avk,
    int iq,
    int * ipa,
    size_t * n0,
    size_t * n1,
    double * cont,
    double * res )
```

Analyze averaging kernels for individual retrieval target.

Definition at line 318 of file retrieval.c.

```
                {

  /* Loop over state vector elements... */
  if (n0[iq] < N)
    for (size_t i = 0; i < n1[iq]; i++) {

      /* Get area of averaging kernel... */
      for (size_t j = 0; j < n1[iq]; j++)
        cont[ipa[n0[iq] + i]] += gsl_matrix_get(avk, n0[iq] + i, n0[iq] + j);

      /* Get information density... */
      res[ipa[n0[iq] + i]] = 1 / gsl_matrix_get(avk, n0[iq] + i, n0[iq] + i);
    }
}
```

5.33.2.3 cost_function()

```
double cost_function (
        gsl_vector * dx,
        gsl_vector * dy,
        gsl_matrix * s_a_inv,
        gsl_vector * sig_eps_inv )
```

Compute cost function.

Definition at line 342 of file retrieval.c.

```
                        {

  gsl_vector *x_aux, *y_aux;

  double chisq_a, chisq_m = 0;

  /* Get sizes... */
  size_t m = dy->size;
  size_t n = dx->size;

  /* Allocate... */
  x_aux = gsl_vector_alloc(n);
  y_aux = gsl_vector_alloc(m);

  /* Determine normalized cost function...
     (chi^2 = 1/m * [dy^T * S_eps^{-1} * dy + dx^T * S_a^{-1} * dx]) */
  for (size_t i = 0; i < m; i++)
    chisq_m += POW2(gsl_vector_get(dy, i) * gsl_vector_get(sig_eps_inv, i));
  gsl_blas_dgemv(CblasNoTrans, 1.0, s_a_inv, dx, 0.0, x_aux);
  gsl_blas_ddot(dx, x_aux, &chisq_a);

  /* Free... */
  gsl_vector_free(x_aux);
  gsl_vector_free(y_aux);

  /* Return cost function value... */
  return (chisq_m + chisq_a) / (double) m;
}
```

5.33.2.4 matrix_invert()

```
void matrix_invert (
        gsl_matrix * a )
```

Invert symmetric matrix.

Definition at line 377 of file retrieval.c.

```
                    {

  size_t diag = 1;

  /* Get size... */
  size_t n = a->size1;

  /* Check if matrix is diagonal... */
  for (size_t i = 0; i < n && diag; i++)
    for (size_t j = i + 1; j < n; j++)
      if (gsl_matrix_get(a, i, j) != 0) {
        diag = 0;
        break;
      }

  /* Quick inversion of diagonal matrix... */
  if (diag)
    for (size_t i = 0; i < n; i++)
      gsl_matrix_set(a, i, i, 1 / gsl_matrix_get(a, i, i));

  /* Matrix inversion by means of Cholesky decomposition... */
  else {
    gsl_linalg_cholesky_decomp(a);
    gsl_linalg_cholesky_invert(a);
  }
}
```

5.33.2.5 matrix_product()

```
void matrix_product (
        gsl_matrix * a,
        gsl_vector * b,
        int transpose,
        gsl_matrix * c )
```

Compute matrix product A^TBA or ABA^T for diagonal matrix B.

Definition at line 407 of file retrieval.c.

```
                     {

  gsl_matrix *aux;

  /* Set sizes... */
  size_t m = a->size1;
  size_t n = a->size2;

  /* Allocate... */
  aux = gsl_matrix_alloc(m, n);

  /* Compute A^T B A... */
  if (transpose == 1) {

    /* Compute B^1/2 A... */
    for (size_t i = 0; i < m; i++)
      for (size_t j = 0; j < n; j++)
        gsl_matrix_set(aux, i, j,
                       gsl_vector_get(b, i) * gsl_matrix_get(a, i, j));

    /* Compute A^T B A = (B^1/2 A)^T (B^1/2 A)... */
    gsl_blas_dgemm(CblasTrans, CblasNoTrans, 1.0, aux, aux, 0.0, c);
  }

  /* Compute A B A^T... */
  else if (transpose == 2) {

    /* Compute A B^1/2... */
    for (size_t i = 0; i < m; i++)
      for (size_t j = 0; j < n; j++)
        gsl_matrix_set(aux, i, j,
                       gsl_matrix_get(a, i, j) * gsl_vector_get(b, j));

    /* Compute A B A^T = (A B^1/2) (A B^1/2)^T... */
    gsl_blas_dgemm(CblasNoTrans, CblasTrans, 1.0, aux, aux, 0.0, c);
  }

  /* Free... */
  gsl_matrix_free(aux);
}
```

5.33.2.6 optimal_estimation()

```
void optimal_estimation (
        ret_t * ret,
        ctl_t * ctl,
        obs_t * obs_meas,
        obs_t * obs_i,
        atm_t * atm_apr,
        atm_t * atm_i )
```

Carry out optimal estimation retrieval.

Definition at line 454 of file retrieval.c.

```
                    {

  static int ipa[N], iqa[N];

  gsl_matrix *a, *auxnm, *corr, *cov, *gain, *k_i, *s_a_inv;
  gsl_vector *b, *dx, *dy, *sig_eps_inv, *sig_formod, *sig_noise,
    *x_a, *x_i, *x_step, *y_aux, *y_i, *y_m;

  FILE *out;

  char filename[2 * LEN];

```

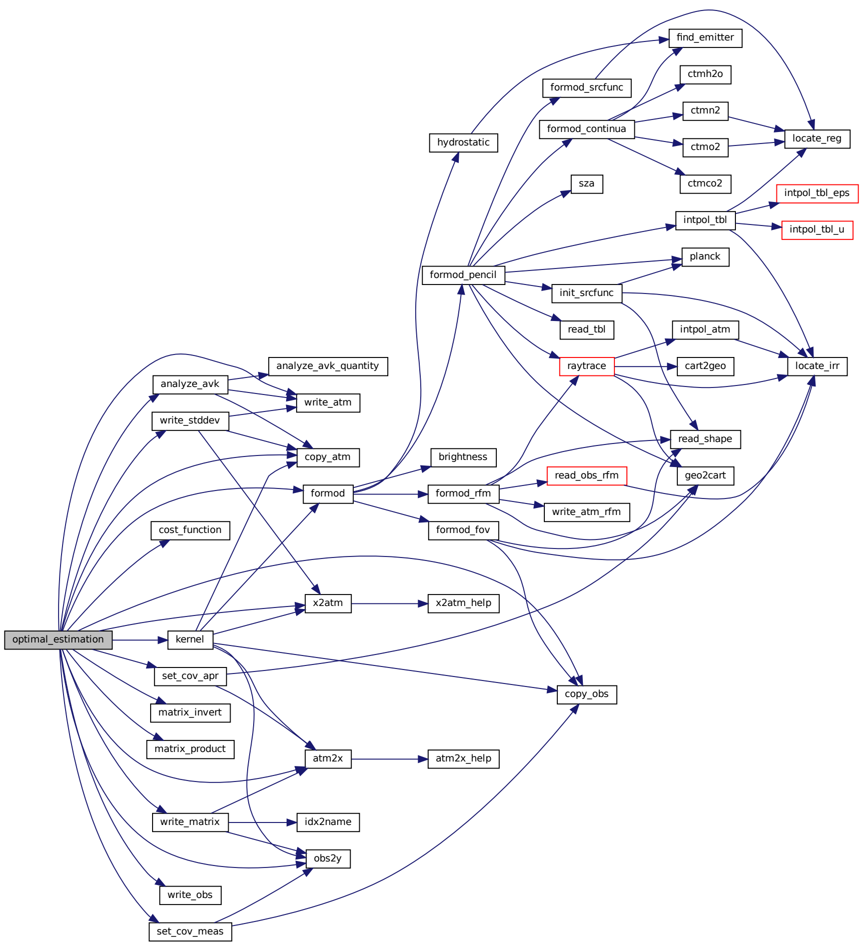
```
double chisq, chisq_old, disq = 0, lmpar = 0.001;

int icl, ig, ip, isf, it = 0, it2, iw;

size_t i, j, m, n;

/* ------------------------------------------------------------
   Initialize...
   ------------------------------------------------------------ */

/* Get sizes... */
m = obs2y(ctl, obs_meas, NULL, NULL, NULL);
n = atm2x(ctl, atm_apr, NULL, iqa, ipa);
if (m == 0 || n == 0)
  ERRMSG("Check problem definition!");

/* Write info... */
LOG(1, "Problem size: m= %d / n= %d "
    "(alloc= %.4g MB / stat= %.4g MB)",
    (int) m, (int) n,
    (double) (3 * m * n + 4 * n * n + 8 * m +
              8 * n) * sizeof(double) / 1024. / 1024.,
    (double) (5 * sizeof(atm_t) + 3 * sizeof(obs_t)
              + 2 * N * sizeof(int)) / 1024. / 1024.);

/* Allocate... */
a = gsl_matrix_alloc(n, n);
cov = gsl_matrix_alloc(n, n);
k_i = gsl_matrix_alloc(m, n);
s_a_inv = gsl_matrix_alloc(n, n);

b = gsl_vector_alloc(n);
dx = gsl_vector_alloc(n);
dy = gsl_vector_alloc(m);
sig_eps_inv = gsl_vector_alloc(m);
sig_formod = gsl_vector_alloc(m);
sig_noise = gsl_vector_alloc(m);
x_a = gsl_vector_alloc(n);
x_i = gsl_vector_alloc(n);
x_step = gsl_vector_alloc(n);
y_aux = gsl_vector_alloc(m);
y_i = gsl_vector_alloc(m);
y_m = gsl_vector_alloc(m);

/* Set initial state... */
copy_atm(ctl, atm_i, atm_apr, 0);
copy_obs(ctl, obs_i, obs_meas, 0);
formod(ctl, atm_i, obs_i);

/* Set state vectors and observation vectors... */
atm2x(ctl, atm_apr, x_a, NULL, NULL);
atm2x(ctl, atm_i, x_i, NULL, NULL);
obs2y(ctl, obs_meas, y_m, NULL, NULL);
obs2y(ctl, obs_i, y_i, NULL, NULL);

/* Set inverse a priori covariance S_a^-1... */
set_cov_apr(ret, ctl, atm_apr, iqa, ipa, s_a_inv);
write_matrix(ret->dir, "matrix_cov_apr.tab", ctl, s_a_inv,
             atm_i, obs_i, "x", "x", "r");
matrix_invert(s_a_inv);

/* Get measurement errors... */
set_cov_meas(ret, ctl, obs_meas, sig_noise, sig_formod, sig_eps_inv);

/* Create cost function file... */
sprintf(filename, "%s/costs.tab", ret->dir);
if (!(out = fopen(filename, "w")))
  ERRMSG("Cannot create cost function file!");

/* Write header... */
fprintf(out,
        "# $1 = iteration number\n"
        "# $2 = normalized cost function\n"
        "# $3 = number of measurements\n"
        "# $4 = number of state vector elements\n\n");

/* Determine dx = x_i - x_a and dy = y - F(x_i) ... */
gsl_vector_memcpy(dx, x_i);
gsl_vector_sub(dx, x_a);
gsl_vector_memcpy(dy, y_m);
gsl_vector_sub(dy, y_i);

/* Compute cost function... */
chisq = cost_function(dx, dy, s_a_inv, sig_eps_inv);

/* Write info... */
LOG(1, "it= %d / chi^2/m= %g", it, chisq);
```

```
  /* Write to cost function file... */
  fprintf(out, "%d %g %d %d\n", it, chisq, (int) m, (int) n);

  /* Compute initial kernel... */
  kernel(ctl, atm_i, obs_i, k_i);

  /* ------------------------------------------------------------
     Levenberg-Marquardt minimization...
     ------------------------------------------------------------ */

  /* Outer loop... */
  for (it = 1; it <= ret->conv_itmax; it++) {

    /* Store current cost function value... */
    chisq_old = chisq;

    /* Compute kernel matrix K_i... */
    if (it > 1 && it % ret->kernel_recomp == 0)
      kernel(ctl, atm_i, obs_i, k_i);

    /* Compute K_i^T * S_eps^{-1} * K_i ... */
    if (it == 1 || it % ret->kernel_recomp == 0)
      matrix_product(k_i, sig_eps_inv, 1, cov);

    /* Determine b = K_i^T * S_eps^{-1} * dy - S_a^{-1} * dx ... */
    for (i = 0; i < m; i++)
      gsl_vector_set(y_aux, i, gsl_vector_get(dy, i)
                     * POW2(gsl_vector_get(sig_eps_inv, i)));
    gsl_blas_dgemv(CblasTrans, 1.0, k_i, y_aux, 0.0, b);
    gsl_blas_dgemv(CblasNoTrans, -1.0, s_a_inv, dx, 1.0, b);

    /* Inner loop... */
    for (it2 = 0; it2 < 20; it2++) {

      /* Compute A = (1 + lmpar) * S_a^{-1} + K_i^T * S_eps^{-1} * K_i ... */
      gsl_matrix_memcpy(a, s_a_inv);
      gsl_matrix_scale(a, 1 + lmpar);
      gsl_matrix_add(a, cov);

      /* Solve A * x_step = b by means of Cholesky decomposition... */
      gsl_linalg_cholesky_decomp(a);
      gsl_linalg_cholesky_solve(a, b, x_step);

      /* Update atmospheric state... */
      gsl_vector_add(x_i, x_step);
      copy_atm(ctl, atm_i, atm_apr, 0);
      copy_obs(ctl, obs_i, obs_meas, 0);
      x2atm(ctl, x_i, atm_i);

      /* Check atmospheric state... */
      for (ip = 0; ip < atm_i->np; ip++) {
        atm_i->p[ip] = GSL_MIN(GSL_MAX(atm_i->p[ip], 5e-7), 5e4);
        atm_i->t[ip] = GSL_MIN(GSL_MAX(atm_i->t[ip], 100), 400);
        for (ig = 0; ig < ctl->ng; ig++)
          atm_i->q[ig][ip] = GSL_MIN(GSL_MAX(atm_i->q[ig][ip], 0), 1);
        for (iw = 0; iw < ctl->nw; iw++)
          atm_i->k[iw][ip] = GSL_MAX(atm_i->k[iw][ip], 0);
      }
      atm_i->clz = GSL_MAX(atm_i->clz, 0);
      atm_i->cldz = GSL_MAX(atm_i->cldz, 0.1);
      for (icl = 0; icl < ctl->ncl; icl++)
        atm_i->clk[icl] = GSL_MAX(atm_i->clk[icl], 0);
      atm_i->sfz = GSL_MAX(atm_i->sfz, 0);
      atm_i->sfp = GSL_MAX(atm_i->sfp, 0);
      atm_i->sft = GSL_MIN(GSL_MAX(atm_i->sft, 100), 400);
      for (isf = 0; isf < ctl->nsf; isf++)
        atm_i->sfeps[isf] = GSL_MIN(GSL_MAX(atm_i->sfeps[isf], 0), 1);

      /* Forward calculation... */
      formod(ctl, atm_i, obs_i);
      obs2y(ctl, obs_i, y_i, NULL, NULL);

      /* Determine dx = x_i - x_a and dy = y - F(x_i) ... */
      gsl_vector_memcpy(dx, x_i);
      gsl_vector_sub(dx, x_a);
      gsl_vector_memcpy(dy, y_m);
      gsl_vector_sub(dy, y_i);

      /* Compute cost function... */
      chisq = cost_function(dx, dy, s_a_inv, sig_eps_inv);

      /* Modify Levenberg-Marquardt parameter... */
      if (chisq > chisq_old) {
        lmpar *= 10;
        gsl_vector_sub(x_i, x_step);
      } else {
```

```
          lmpar /= 10;
          break;
        }
      }

      /* Write info... */
      LOG(1, "it= %d / chi^2/m= %g", it, chisq);

      /* Write to cost function file... */
      fprintf(out, "%d %g %d %d\n", it, chisq, (int) m, (int) n);

      /* Get normalized step size in state space... */
      gsl_blas_ddot(x_step, b, &disq);
      disq /= (double) n;

      /* Convergence test... */
      if ((it == 1 || it % ret->kernel_recomp == 0) && disq < ret->conv_dmin)
        break;
    }

    /* Close cost function file... */
    fclose(out);

    /* Store results... */
    write_atm(ret->dir, "atm_final.tab", ctl, atm_i);
    write_obs(ret->dir, "obs_final.tab", ctl, obs_i);
    write_matrix(ret->dir, "matrix_kernel.tab", ctl, k_i,
                 atm_i, obs_i, "y", "x", "r");

    /* ------------------------------------------------------------
       Analysis of retrieval results...
       ------------------------------------------------------------ */

    /* Check if error analysis is requested... */
    if (ret->err_ana) {

      /* Allocate... */
      auxnm = gsl_matrix_alloc(n, m);
      corr = gsl_matrix_alloc(n, n);
      gain = gsl_matrix_alloc(n, m);

      /* Compute inverse retrieval covariance...
         cov^{-1} = S_a^{-1} + K_i^T * S_eps^{-1} * K_i */
      matrix_product(k_i, sig_eps_inv, 1, cov);
      gsl_matrix_add(cov, s_a_inv);

      /* Compute retrieval covariance... */
      matrix_invert(cov);
      write_matrix(ret->dir, "matrix_cov_ret.tab", ctl, cov,
                   atm_i, obs_i, "x", "x", "r");
      write_stddev("total", ret, ctl, atm_i, cov);

      /* Compute correlation matrix... */
      for (i = 0; i < n; i++)
        for (j = 0; j < n; j++)
          gsl_matrix_set(corr, i, j, gsl_matrix_get(cov, i, j)
                         / sqrt(gsl_matrix_get(cov, i, i))
                         / sqrt(gsl_matrix_get(cov, j, j)));
      write_matrix(ret->dir, "matrix_corr.tab", ctl, corr,
                   atm_i, obs_i, "x", "x", "r");

      /* Compute gain matrix...
         G = cov * K^T * S_eps^{-1} */
      for (i = 0; i < n; i++)
        for (j = 0; j < m; j++)
          gsl_matrix_set(auxnm, i, j, gsl_matrix_get(k_i, j, i)
                         * POW2(gsl_vector_get(sig_eps_inv, j)));
      gsl_blas_dgemm(CblasNoTrans, CblasNoTrans, 1.0, cov, auxnm, 0.0, gain);
      write_matrix(ret->dir, "matrix_gain.tab", ctl, gain,
                   atm_i, obs_i, "x", "y", "c");

      /* Compute retrieval error due to noise... */
      matrix_product(gain, sig_noise, 2, a);
      write_stddev("noise", ret, ctl, atm_i, a);

      /* Compute retrieval error  due to forward model errors... */
      matrix_product(gain, sig_formod, 2, a);
      write_stddev("formod", ret, ctl, atm_i, a);

      /* Compute averaging kernel matrix
         A = G * K ... */
      gsl_blas_dgemm(CblasNoTrans, CblasNoTrans, 1.0, gain, k_i, 0.0, a);
      write_matrix(ret->dir, "matrix_avk.tab", ctl, a,
                   atm_i, obs_i, "x", "x", "r");

      /* Analyze averaging kernel matrix... */
      analyze_avk(ret, ctl, atm_i, iqa, ipa, a);
```

```
    /* Free... */
    gsl_matrix_free(auxnm);
    gsl_matrix_free(corr);
    gsl_matrix_free(gain);
  }

  /* ------------------------------------------------------------
     Finalize...
     ------------------------------------------------------------ */

  gsl_matrix_free(a);
  gsl_matrix_free(cov);
  gsl_matrix_free(k_i);
  gsl_matrix_free(s_a_inv);

  gsl_vector_free(b);
  gsl_vector_free(dx);
  gsl_vector_free(dy);
  gsl_vector_free(sig_eps_inv);
  gsl_vector_free(sig_formod);
  gsl_vector_free(sig_noise);
  gsl_vector_free(x_a);
  gsl_vector_free(x_i);
  gsl_vector_free(x_step);
  gsl_vector_free(y_aux);
  gsl_vector_free(y_i);
  gsl_vector_free(y_m);
}
```

Here is the call graph for this function:



5.33.2.7 read_ret()

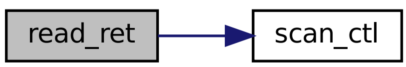
```
void read_ret (
        int argc,
        char * argv[],
        ctl_t * ctl,
        ret_t * ret )
```

Read retrieval control parameters.

Definition at line 765 of file retrieval.c.

```
                {

  /* Iteration control... */
  ret->kernel_recomp =
    (int) scan_ctl(argc, argv, "KERNEL_RECOMP", -1, "3", NULL);
  ret->conv_itmax = (int) scan_ctl(argc, argv, "CONV_ITMAX", -1, "30", NULL);
  ret->conv_dmin = scan_ctl(argc, argv, "CONV_DMIN", -1, "0.1", NULL);

  /* Error analysis... */
  ret->err_ana = (int) scan_ctl(argc, argv, "ERR_ANA", -1, "1", NULL);

  for (int id = 0; id < ctl->nd; id++)
    ret->err_formod[id] = scan_ctl(argc, argv, "ERR_FORMOD", id, "0", NULL);

  for (int id = 0; id < ctl->nd; id++)
    ret->err_noise[id] = scan_ctl(argc, argv, "ERR_NOISE", id, "0", NULL);

  ret->err_press = scan_ctl(argc, argv, "ERR_PRESS", -1, "0", NULL);
  ret->err_press_cz = scan_ctl(argc, argv, "ERR_PRESS_CZ", -1, "-999", NULL);
  ret->err_press_ch = scan_ctl(argc, argv, "ERR_PRESS_CH", -1, "-999", NULL);

  ret->err_temp = scan_ctl(argc, argv, "ERR_TEMP", -1, "0", NULL);
  ret->err_temp_cz = scan_ctl(argc, argv, "ERR_TEMP_CZ", -1, "-999", NULL);
  ret->err_temp_ch = scan_ctl(argc, argv, "ERR_TEMP_CH", -1, "-999", NULL);

  for (int ig = 0; ig < ctl->ng; ig++) {
    ret->err_q[ig] = scan_ctl(argc, argv, "ERR_Q", ig, "0", NULL);
    ret->err_q_cz[ig] = scan_ctl(argc, argv, "ERR_Q_CZ", ig, "-999", NULL);
    ret->err_q_ch[ig] = scan_ctl(argc, argv, "ERR_Q_CH", ig, "-999", NULL);
  }

  for (int iw = 0; iw < ctl->nw; iw++) {
    ret->err_k[iw] = scan_ctl(argc, argv, "ERR_K", iw, "0", NULL);
    ret->err_k_cz[iw] = scan_ctl(argc, argv, "ERR_K_CZ", iw, "-999", NULL);
    ret->err_k_ch[iw] = scan_ctl(argc, argv, "ERR_K_CH", iw, "-999", NULL);
  }

  ret->err_clz = scan_ctl(argc, argv, "ERR_CLZ", -1, "0", NULL);
  ret->err_cldz = scan_ctl(argc, argv, "ERR_CLDZ", -1, "0", NULL);
  for (int icl = 0; icl < ctl->ncl; icl++)
    ret->err_clk[icl] = scan_ctl(argc, argv, "ERR_CLK", icl, "0", NULL);

  ret->err_sfz = scan_ctl(argc, argv, "ERR_SFZ", -1, "0", NULL);
  ret->err_sfp = scan_ctl(argc, argv, "ERR_SFP", -1, "0", NULL);
  ret->err_sft = scan_ctl(argc, argv, "ERR_SFT", -1, "0", NULL);
  for (int isf = 0; isf < ctl->nsf; isf++)
    ret->err_sfeps[isf] = scan_ctl(argc, argv, "ERR_SFEPS", isf, "0", NULL);
}
```

Here is the call graph for this function:



5.33.2.8 set_cov_apr()

```
void set_cov_apr (
        ret_t * ret,
        ctl_t * ctl,
        atm_t * atm,
        int * iqa,
        int * ipa,
        gsl_matrix * s_a )
```

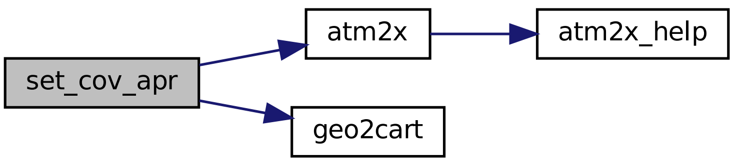
Set a priori covariance.

Definition at line 820 of file retrieval.c.

```
                  {

  gsl_vector *x_a;

  double x0[3], x1[3];

  /* Get sizes... */
  size_t n = s_a->size1;

  /* Allocate... */
  x_a = gsl_vector_alloc(n);

  /* Get sigma vector... */
  atm2x(ctl, atm, x_a, NULL, NULL);
  for (size_t i = 0; i < n; i++) {
    if (iqa[i] == IDXP)
      gsl_vector_set(x_a, i, ret->err_press / 100 * gsl_vector_get(x_a, i));
    if (iqa[i] == IDXT)
      gsl_vector_set(x_a, i, ret->err_temp);
    for (int ig = 0; ig < ctl->ng; ig++)
      if (iqa[i] == IDXQ(ig))
        gsl_vector_set(x_a, i, ret->err_q[ig] / 100 * gsl_vector_get(x_a, i));
    for (int iw = 0; iw < ctl->nw; iw++)
      if (iqa[i] == IDXK(iw))
        gsl_vector_set(x_a, i, ret->err_k[iw]);
    if (iqa[i] == IDXCLZ)
      gsl_vector_set(x_a, i, ret->err_clz);
    if (iqa[i] == IDXCLDZ)
      gsl_vector_set(x_a, i, ret->err_cldz);
    for (int icl = 0; icl < ctl->ncl; icl++)
      if (iqa[i] == IDXCLK(icl))
        gsl_vector_set(x_a, i, ret->err_clk[icl]);
    if (iqa[i] == IDXSFZ)
      gsl_vector_set(x_a, i, ret->err_sfz);
    if (iqa[i] == IDXSFP)
      gsl_vector_set(x_a, i, ret->err_sfp);
    if (iqa[i] == IDXSFT)
      gsl_vector_set(x_a, i, ret->err_sft);
    for (int isf = 0; isf < ctl->nsf; isf++)
      if (iqa[i] == IDXSFEPS(isf))
        gsl_vector_set(x_a, i, ret->err_sfeps[isf]);
  }

  /* Check standard deviations... */
  for (size_t i = 0; i < n; i++)
    if (POW2(gsl_vector_get(x_a, i)) <= 0)
      ERRMSG("Check a priori data (zero standard deviation)!");

  /* Initialize diagonal covariance... */
  gsl_matrix_set_zero(s_a);
  for (size_t i = 0; i < n; i++)
    gsl_matrix_set(s_a, i, i, POW2(gsl_vector_get(x_a, i)));

  /* Loop over matrix elements... */
  for (size_t i = 0; i < n; i++)
    for (size_t j = 0; j < n; j++)
      if (i != j && iqa[i] == iqa[j]) {

        /* Initialize... */
        double cz = 0;
        double ch = 0;

        /* Set correlation lengths for pressure... */
        if (iqa[i] == IDXP) {
          cz = ret->err_press_cz;
          ch = ret->err_press_ch;
        }

        /* Set correlation lengths for temperature... */
        if (iqa[i] == IDXT) {
          cz = ret->err_temp_cz;
```

```
          ch = ret->err_temp_ch;
        }

        /* Set correlation lengths for volume mixing ratios... */
        for (int ig = 0; ig < ctl->ng; ig++)
          if (iqa[i] == IDXQ(ig)) {
            cz = ret->err_q_cz[ig];
            ch = ret->err_q_ch[ig];
          }

        /* Set correlation lengths for extinction... */
        for (int iw = 0; iw < ctl->nw; iw++)
          if (iqa[i] == IDXK(iw)) {
            cz = ret->err_k_cz[iw];
            ch = ret->err_k_ch[iw];
          }

        /* Compute correlations... */
        if (cz > 0 && ch > 0) {

          /* Get Cartesian coordinates... */
          geo2cart(0, atm->lon[ipa[i]], atm->lat[ipa[i]], x0);
          geo2cart(0, atm->lon[ipa[j]], atm->lat[ipa[j]], x1);

          /* Compute correlations... */
          double rho =
            exp(-DIST(x0, x1) / ch -
                fabs(atm->z[ipa[i]] - atm->z[ipa[j]]) / cz);

          /* Set covariance... */
          gsl_matrix_set(s_a, i, j, gsl_vector_get(x_a, i)
                         * gsl_vector_get(x_a, j) * rho);
        }
      }

  /* Free... */
  gsl_vector_free(x_a);
}
```

Here is the call graph for this function:



5.33.2.9 set_cov_meas()

```
void set_cov_meas (
    ret_t * ret,
    ctl_t * ctl,
    obs_t * obs,
    gsl_vector * sig_noise,
    gsl_vector * sig_formod,
    gsl_vector * sig_eps_inv )
```

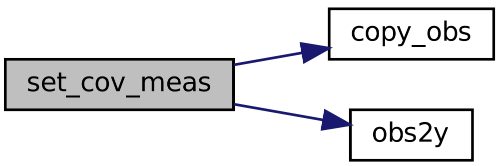
Set measurement errors.

Definition at line 938 of file retrieval.c.

```
                                 {

```

```
  static obs_t obs_err;

  /* Get size... */
  size_t m = sig_eps_inv->size;

  /* Noise error (always considered in retrieval fit)... */
  copy_obs(ctl, &obs_err, obs, 1);
  for (int ir = 0; ir < obs_err.nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      obs_err.rad[id][ir]
        = (gsl_finite(obs->rad[id][ir]) ? ret->err_noise[id] : GSL_NAN);
  obs2y(ctl, &obs_err, sig_noise, NULL, NULL);

  /* Forward model error (always considered in retrieval fit)... */
  copy_obs(ctl, &obs_err, obs, 1);
  for (int ir = 0; ir < obs_err.nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      obs_err.rad[id][ir]
        = fabs(ret->err_formod[id] / 100 * obs->rad[id][ir]);
  obs2y(ctl, &obs_err, sig_formod, NULL, NULL);

  /* Total error... */
  for (size_t i = 0; i < m; i++)
    gsl_vector_set(sig_eps_inv, i, 1 / sqrt(POW2(gsl_vector_get(sig_noise, i))
                                            +
                                            POW2(gsl_vector_get
                                                 (sig_formod, i))));

  /* Check standard deviations... */
  for (size_t i = 0; i < m; i++)
    if (gsl_vector_get(sig_eps_inv, i) <= 0)
      ERRMSG("Check measurement errors (zero standard deviation)!");
}
```

Here is the call graph for this function:



5.33.2.10 write_stddev()

```
void write_stddev (
    const char * quantity,
    ret_t * ret,
    ctl_t * ctl,
    atm_t * atm,
    gsl_matrix * s )
```

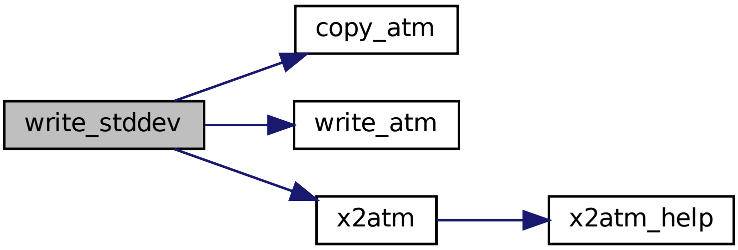
Write retrieval error to file.

Definition at line 982 of file retrieval.c.

```
                   {

  static atm_t atm_aux;

  gsl_vector *x_aux;

  char filename[LEN];

```

```
  /* Get sizes... */
  size_t n = s->size1;

  /* Allocate... */
  x_aux = gsl_vector_alloc(n);

  /* Compute standard deviation... */
  for (size_t i = 0; i < n; i++)
    gsl_vector_set(x_aux, i, sqrt(gsl_matrix_get(s, i, i)));

  /* Write to disk... */
  copy_atm(ctl, &atm_aux, atm, 1);
  x2atm(ctl, x_aux, &atm_aux);
  sprintf(filename, "atm_err_%s.tab", quantity);
  write_atm(ret->dir, filename, ctl, &atm_aux);

  /* Free... */
  gsl_vector_free(x_aux);
}
```

Here is the call graph for this function:



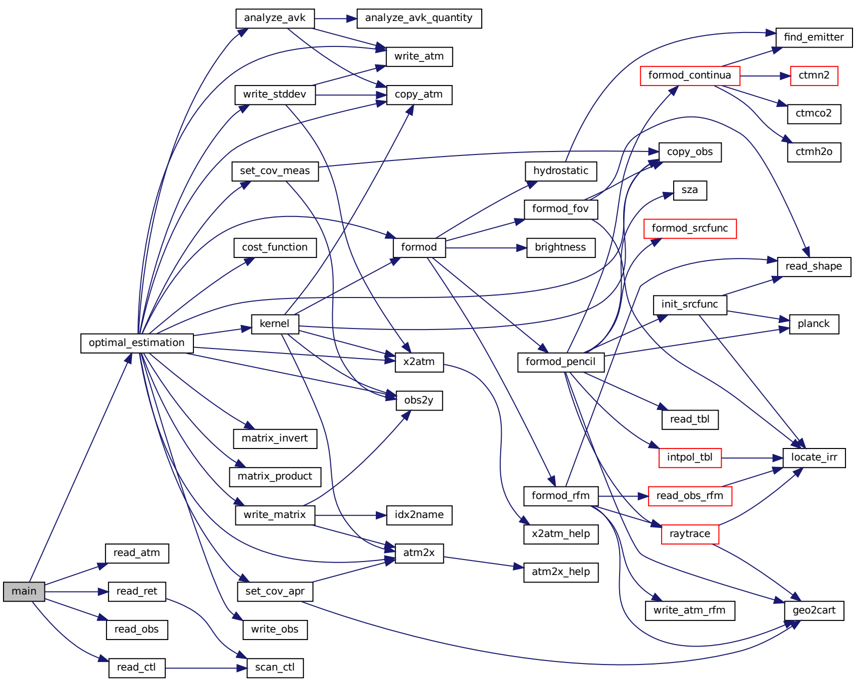
5.33.2.11 main() int main (int *argc*, char * *argv[ ]*)

Definition at line 201 of file retrieval.c.

```
                  {

  static atm_t atm_i, atm_apr;
  static ctl_t ctl;
  static obs_t obs_i, obs_meas;
  static ret_t ret;

  FILE *dirlist;

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <dirlist>");

  /* Measure CPU-time... */
  TIMER("total", 1);

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  read_ret(argc, argv, &ctl, &ret);

  /* Open directory list... */
  if (!(dirlist = fopen(argv[2], "r")))
    ERRMSG("Cannot open directory list!");

  /* Loop over directories... */
  while (fscanf(dirlist, "%s", ret.dir) != EOF) {
```

```
    /* Write info... */
    LOG(1, "\nRetrieve in directory %s...\n", ret.dir);

    /* Read atmospheric data... */
    read_atm(ret.dir, "atm_apr.tab", &ctl, &atm_apr);

    /* Read observation data... */
    read_obs(ret.dir, "obs_meas.tab", &ctl, &obs_meas);

    /* Run retrieval... */
    optimal_estimation(&ret, &ctl, &obs_meas, &obs_i, &atm_apr, &atm_i);

    /* Measure CPU-time... */
    TIMER("total", 2);
  }

  /* Write info... */
  LOG(1, "\nRetrieval done...");

  /* Measure CPU-time... */
  TIMER("total", 3);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.34 retrieval.c

```
/*
  This file is part of JURASSIC.

  JURASSIC is free software: you can redistribute it and/or modify
  it under the terms of the GNU General Public License as published by
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```

```
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*/

#include "jurassic.h"

/* ------------------------------------------------------------
   Structs...
   ------------------------------------------------------------ */

typedef struct {

  char dir[LEN];

  int kernel_recomp;

  int conv_itmax;

  double conv_dmin;

  int err_ana;

  double err_formod[ND];

  double err_noise[ND];

  double err_press;

  double err_press_cz;

  double err_press_ch;

  double err_temp;

  double err_temp_cz;

  double err_temp_ch;

  double err_q[NG];

  double err_q_cz[NG];

  double err_q_ch[NG];

  double err_k[NW];

  double err_k_cz[NW];

  double err_k_ch[NW];

  double err_clz;

  double err_cldz;

  double err_clk[NCL];

  double err_sfz;

  double err_sfp;

  double err_sft;

  double err_sfeps[NSF];

} ret_t;

/* ------------------------------------------------------------
   Functions...
   ------------------------------------------------------------ */

void analyze_avk(
  ret_t * ret,
  ctl_t * ctl,
  atm_t * atm,
  int *iqa,
  int *ipa,
  gsl_matrix * avk);

void analyze_avk_quantity(
  gsl_matrix * avk,
  int iq,
  int *ipa,
  size_t *n0,
  size_t *n1,
  double *cont,
  double *res);

```

```
double cost_function(
  gsl_vector * dx,
  gsl_vector * dy,
  gsl_matrix * s_a_inv,
  gsl_vector * sig_eps_inv);

void matrix_invert(
  gsl_matrix * a);

void matrix_product(
  gsl_matrix * a,
  gsl_vector * b,
  int transpose,
  gsl_matrix * c);

void optimal_estimation(
  ret_t * ret,
  ctl_t * ctl,
  obs_t * obs_meas,
  obs_t * obs_i,
  atm_t * atm_apr,
  atm_t * atm_i);

void read_ret(
  int argc,
  char *argv[],
  ctl_t * ctl,
  ret_t * ret);

void set_cov_apr(
  ret_t * ret,
  ctl_t * ctl,
  atm_t * atm,
  int *iqa,
  int *ipa,
  gsl_matrix * s_a);

void set_cov_meas(
  ret_t * ret,
  ctl_t * ctl,
  obs_t * obs,
  gsl_vector * sig_noise,
  gsl_vector * sig_formod,
  gsl_vector * sig_eps_inv);

void write_stddev(
  const char *quantity,
  ret_t * ret,
  ctl_t * ctl,
  atm_t * atm,
  gsl_matrix * s);

/* ------------------------------------------------------------
   Main...
   ------------------------------------------------------------ */

int main(
  int argc,
  char *argv[]) {

  static atm_t atm_i, atm_apr;
  static ctl_t ctl;
  static obs_t obs_i, obs_meas;
  static ret_t ret;

  FILE *dirlist;

  /* Check arguments... */
  if (argc < 3)
    ERRMSG("Give parameters: <ctl> <dirlist>");

  /* Measure CPU-time... */
  TIMER("total", 1);

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);
  read_ret(argc, argv, &ctl, &ret);

  /* Open directory list... */
  if (!(dirlist = fopen(argv[2], "r")))
    ERRMSG("Cannot open directory list!");

  /* Loop over directories... */
  while (fscanf(dirlist, "%s", ret.dir) != EOF) {

    /* Write info... */
    LOG(1, "\nRetrieve in directory %s...\n", ret.dir);
```

```

    /* Read atmospheric data... */
    read_atm(ret.dir, "atm_apr.tab", &ctl, &atm_apr);

    /* Read observation data... */
    read_obs(ret.dir, "obs_meas.tab", &ctl, &obs_meas);

    /* Run retrieval... */
    optimal_estimation(&ret, &ctl, &obs_meas, &obs_i, &atm_apr, &atm_i);

    /* Measure CPU-time... */
    TIMER("total", 2);
  }

  /* Write info... */
  LOG(1, "\nRetrieval done...");

  /* Measure CPU-time... */
  TIMER("total", 3);

  return EXIT_SUCCESS;
}

/*****************************************************************************/

void analyze_avk(
  ret_t * ret,
  ctl_t * ctl,
  atm_t * atm,
  int *iqa,
  int *ipa,
  gsl_matrix * avk) {

  static atm_t atm_cont, atm_res;

  int icl, ig, iq, isf, iw;

  size_t i, n, n0[NQ], n1[NQ];

  /* Get sizes... */
  n = avk->size1;

  /* Find sub-matrices for different quantities... */
  for (iq = 0; iq < NQ; iq++) {
    n0[iq] = N;
    for (i = 0; i < n; i++) {
      if (iqa[i] == iq && n0[iq] == N)
        n0[iq] = i;
      if (iqa[i] == iq)
        n1[iq] = i - n0[iq] + 1;
    }
  }

  /* Initialize... */
  copy_atm(ctl, &atm_cont, atm, 1);
  copy_atm(ctl, &atm_res, atm, 1);

  /* Analyze quantities... */
  analyze_avk_quantity(avk, IDXP, ipa, n0, n1, atm_cont.p, atm_res.p);
  analyze_avk_quantity(avk, IDXT, ipa, n0, n1, atm_cont.t, atm_res.t);
  for (ig = 0; ig < ctl->ng; ig++)
    analyze_avk_quantity(avk, IDXQ(ig), ipa, n0, n1,
                         atm_cont.q[ig], atm_res.q[ig]);
  for (iw = 0; iw < ctl->nw; iw++)
    analyze_avk_quantity(avk, IDXK(iw), ipa, n0, n1,
                         atm_cont.k[iw], atm_res.k[iw]);
  analyze_avk_quantity(avk, IDXCLZ, ipa, n0, n1, &atm_cont.clz, &atm_res.clz);
  analyze_avk_quantity(avk, IDXCLDZ, ipa, n0, n1, &atm_cont.cldz,
                       &atm_res.cldz);
  for (icl = 0; icl < ctl->ncl; icl++)
    analyze_avk_quantity(avk, IDXCLK(icl), ipa, n0, n1,
                         &atm_cont.clk[icl], &atm_res.clk[icl]);
  analyze_avk_quantity(avk, IDXSFZ, ipa, n0, n1, &atm_cont.sfz, &atm_res.sfz);
  analyze_avk_quantity(avk, IDXSFP, ipa, n0, n1, &atm_cont.sfp, &atm_res.sfp);
  analyze_avk_quantity(avk, IDXSFT, ipa, n0, n1, &atm_cont.sft, &atm_res.sft);
  for (isf = 0; isf < ctl->nsf; isf++)
    analyze_avk_quantity(avk, IDXSFEPS(isf), ipa, n0, n1,
                         &atm_cont.sfeps[isf], &atm_res.sfeps[isf]);

  /* Write results to disk... */
  write_atm(ret->dir, "atm_cont.tab", ctl, &atm_cont);
  write_atm(ret->dir, "atm_res.tab", ctl, &atm_res);
}

/*****************************************************************************/

void analyze_avk_quantity(
```

```
  gsl_matrix * avk,
  int iq,
  int *ipa,
  size_t *n0,
  size_t *n1,
  double *cont,
  double *res) {

  /* Loop over state vector elements... */
  if (n0[iq] < N)
    for (size_t i = 0; i < n1[iq]; i++) {

      /* Get area of averaging kernel... */
      for (size_t j = 0; j < n1[iq]; j++)
        cont[ipa[n0[iq] + i]] += gsl_matrix_get(avk, n0[iq] + i, n0[iq] + j);

      /* Get information density... */
      res[ipa[n0[iq] + i]] = 1 / gsl_matrix_get(avk, n0[iq] + i, n0[iq] + i);
    }
}

/*****************************************************************************/

double cost_function(
  gsl_vector * dx,
  gsl_vector * dy,
  gsl_matrix * s_a_inv,
  gsl_vector * sig_eps_inv) {

  gsl_vector *x_aux, *y_aux;

  double chisq_a, chisq_m = 0;

  /* Get sizes... */
  size_t m = dy->size;
  size_t n = dx->size;

  /* Allocate... */
  x_aux = gsl_vector_alloc(n);
  y_aux = gsl_vector_alloc(m);

  /* Determine normalized cost function...
     (chi^2 = 1/m * [dy^T * S_eps^{-1} * dy + dx^T * S_a^{-1} * dx]) */
  for (size_t i = 0; i < m; i++)
    chisq_m += POW2(gsl_vector_get(dy, i) * gsl_vector_get(sig_eps_inv, i));
  gsl_blas_dgemv(CblasNoTrans, 1.0, s_a_inv, dx, 0.0, x_aux);
  gsl_blas_ddot(dx, x_aux, &chisq_a);

  /* Free... */
  gsl_vector_free(x_aux);
  gsl_vector_free(y_aux);

  /* Return cost function value... */
  return (chisq_m + chisq_a) / (double) m;
}

/*****************************************************************************/

void matrix_invert(
  gsl_matrix * a) {

  size_t diag = 1;

  /* Get size... */
  size_t n = a->size1;

  /* Check if matrix is diagonal... */
  for (size_t i = 0; i < n && diag; i++)
    for (size_t j = i + 1; j < n; j++)
      if (gsl_matrix_get(a, i, j) != 0) {
        diag = 0;
        break;
      }

  /* Quick inversion of diagonal matrix... */
  if (diag)
    for (size_t i = 0; i < n; i++)
      gsl_matrix_set(a, i, i, 1 / gsl_matrix_get(a, i, i));

  /* Matrix inversion by means of Cholesky decomposition... */
  else {
    gsl_linalg_cholesky_decomp(a);
    gsl_linalg_cholesky_invert(a);
  }
}

/*****************************************************************************/
```

```
void matrix_product(
  gsl_matrix * a,
  gsl_vector * b,
  int transpose,
  gsl_matrix * c) {

  gsl_matrix *aux;

  /* Set sizes... */
  size_t m = a->size1;
  size_t n = a->size2;

  /* Allocate... */
  aux = gsl_matrix_alloc(m, n);

  /* Compute A^T B A... */
  if (transpose == 1) {

    /* Compute B^1/2 A... */
    for (size_t i = 0; i < m; i++)
      for (size_t j = 0; j < n; j++)
        gsl_matrix_set(aux, i, j,
                       gsl_vector_get(b, i) * gsl_matrix_get(a, i, j));

    /* Compute A^T B A = (B^1/2 A)^T (B^1/2 A)... */
    gsl_blas_dgemm(CblasTrans, CblasNoTrans, 1.0, aux, aux, 0.0, c);
  }

  /* Compute A B A^T... */
  else if (transpose == 2) {

    /* Compute A B^1/2... */
    for (size_t i = 0; i < m; i++)
      for (size_t j = 0; j < n; j++)
        gsl_matrix_set(aux, i, j,
                       gsl_matrix_get(a, i, j) * gsl_vector_get(b, j));

    /* Compute A B A^T = (A B^1/2) (A B^1/2)^T... */
    gsl_blas_dgemm(CblasNoTrans, CblasTrans, 1.0, aux, aux, 0.0, c);
  }

  /* Free... */
  gsl_matrix_free(aux);
}

/*****************************************************************************/

void optimal_estimation(
  ret_t * ret,
  ctl_t * ctl,
  obs_t * obs_meas,
  obs_t * obs_i,
  atm_t * atm_apr,
  atm_t * atm_i) {

  static int ipa[N], iqa[N];

  gsl_matrix *a, *auxnm, *corr, *cov, *gain, *k_i, *s_a_inv;
  gsl_vector *b, *dx, *dy, *sig_eps_inv, *sig_formod, *sig_noise,
    *x_a, *x_i, *x_step, *y_aux, *y_i, *y_m;

  FILE *out;

  char filename[2 * LEN];

  double chisq, chisq_old, disq = 0, lmpar = 0.001;

  int icl, ig, ip, isf, it = 0, it2, iw;

  size_t i, j, m, n;

  /* ------------------------------------------------------------
     Initialize...
     ------------------------------------------------------------ */

  /* Get sizes... */
  m = obs2y(ctl, obs_meas, NULL, NULL, NULL);
  n = atm2x(ctl, atm_apr, NULL, iqa, ipa);
  if (m == 0 || n == 0)
    ERRMSG("Check problem definition!");

  /* Write info... */
  LOG(1, "Problem size: m= %d / n= %d "
      "(alloc= %.4g MB / stat= %.4g MB)",
      (int) m, (int) n,
      (double) (3 * m * n + 4 * n * n + 8 * m +
```

```
               8 * n) * sizeof(double) / 1024. / 1024.,
        (double) (5 * sizeof(atm_t) + 3 * sizeof(obs_t)
               + 2 * N * sizeof(int)) / 1024. / 1024.);

  /* Allocate... */
  a = gsl_matrix_alloc(n, n);
  cov = gsl_matrix_alloc(n, n);
  k_i = gsl_matrix_alloc(m, n);
  s_a_inv = gsl_matrix_alloc(n, n);

  b = gsl_vector_alloc(n);
  dx = gsl_vector_alloc(n);
  dy = gsl_vector_alloc(m);
  sig_eps_inv = gsl_vector_alloc(m);
  sig_formod = gsl_vector_alloc(m);
  sig_noise = gsl_vector_alloc(m);
  x_a = gsl_vector_alloc(n);
  x_i = gsl_vector_alloc(n);
  x_step = gsl_vector_alloc(n);
  y_aux = gsl_vector_alloc(m);
  y_i = gsl_vector_alloc(m);
  y_m = gsl_vector_alloc(m);

  /* Set initial state... */
  copy_atm(ctl, atm_i, atm_apr, 0);
  copy_obs(ctl, obs_i, obs_meas, 0);
  formod(ctl, atm_i, obs_i);

  /* Set state vectors and observation vectors... */
  atm2x(ctl, atm_apr, x_a, NULL, NULL);
  atm2x(ctl, atm_i, x_i, NULL, NULL);
  obs2y(ctl, obs_meas, y_m, NULL, NULL);
  obs2y(ctl, obs_i, y_i, NULL, NULL);

  /* Set inverse a priori covariance S_a^-1... */
  set_cov_apr(ret, ctl, atm_apr, iqa, ipa, s_a_inv);
  write_matrix(ret->dir, "matrix_cov_apr.tab", ctl, s_a_inv,
               atm_i, obs_i, "x", "x", "r");
  matrix_invert(s_a_inv);

  /* Get measurement errors... */
  set_cov_meas(ret, ctl, obs_meas, sig_noise, sig_formod, sig_eps_inv);

  /* Create cost function file... */
  sprintf(filename, "%s/costs.tab", ret->dir);
  if (!(out = fopen(filename, "w")))
    ERRMSG("Cannot create cost function file!");

  /* Write header... */
  fprintf(out,
          "# $1 = iteration number\n"
          "# $2 = normalized cost function\n"
          "# $3 = number of measurements\n"
          "# $4 = number of state vector elements\n\n");

  /* Determine dx = x_i - x_a and dy = y - F(x_i) ... */
  gsl_vector_memcpy(dx, x_i);
  gsl_vector_sub(dx, x_a);
  gsl_vector_memcpy(dy, y_m);
  gsl_vector_sub(dy, y_i);

  /* Compute cost function... */
  chisq = cost_function(dx, dy, s_a_inv, sig_eps_inv);

  /* Write info... */
  LOG(1, "it= %d / chi^2/m= %g", it, chisq);

  /* Write to cost function file... */
  fprintf(out, "%d %g %d %d\n", it, chisq, (int) m, (int) n);

  /* Compute initial kernel... */
  kernel(ctl, atm_i, obs_i, k_i);

  /* ------------------------------------------------------------
     Levenberg-Marquardt minimization...
     ------------------------------------------------------------ */

  /* Outer loop... */
  for (it = 1; it <= ret->conv_itmax; it++) {

    /* Store current cost function value... */
    chisq_old = chisq;

    /* Compute kernel matrix K_i... */
    if (it > 1 && it % ret->kernel_recomp == 0)
      kernel(ctl, atm_i, obs_i, k_i);

```

```
    /* Compute K_i^T * S_eps^{-1} * K_i ... */
    if (it == 1 || it % ret->kernel_recomp == 0)
      matrix_product(k_i, sig_eps_inv, 1, cov);

    /* Determine b = K_i^T * S_eps^{-1} * dy - S_a^{-1} * dx ... */
    for (i = 0; i < m; i++)
      gsl_vector_set(y_aux, i, gsl_vector_get(dy, i)
                     * POW2(gsl_vector_get(sig_eps_inv, i)));
    gsl_blas_dgemv(CblasTrans, 1.0, k_i, y_aux, 0.0, b);
    gsl_blas_dgemv(CblasNoTrans, -1.0, s_a_inv, dx, 1.0, b);

    /* Inner loop... */
    for (it2 = 0; it2 < 20; it2++) {

      /* Compute A = (1 + lmpar) * S_a^{-1} + K_i^T * S_eps^{-1} * K_i ... */
      gsl_matrix_memcpy(a, s_a_inv);
      gsl_matrix_scale(a, 1 + lmpar);
      gsl_matrix_add(a, cov);

      /* Solve A * x_step = b by means of Cholesky decomposition... */
      gsl_linalg_cholesky_decomp(a);
      gsl_linalg_cholesky_solve(a, b, x_step);

      /* Update atmospheric state... */
      gsl_vector_add(x_i, x_step);
      copy_atm(ctl, atm_i, atm_apr, 0);
      copy_obs(ctl, obs_i, obs_meas, 0);
      x2atm(ctl, x_i, atm_i);

      /* Check atmospheric state... */
      for (ip = 0; ip < atm_i->np; ip++) {
        atm_i->p[ip] = GSL_MIN(GSL_MAX(atm_i->p[ip], 5e-7), 5e4);
        atm_i->t[ip] = GSL_MIN(GSL_MAX(atm_i->t[ip], 100), 400);
        for (ig = 0; ig < ctl->ng; ig++)
          atm_i->q[ig][ip] = GSL_MIN(GSL_MAX(atm_i->q[ig][ip], 0), 1);
        for (iw = 0; iw < ctl->nw; iw++)
          atm_i->k[iw][ip] = GSL_MAX(atm_i->k[iw][ip], 0);
      }
      atm_i->clz = GSL_MAX(atm_i->clz, 0);
      atm_i->cldz = GSL_MAX(atm_i->cldz, 0.1);
      for (icl = 0; icl < ctl->ncl; icl++)
        atm_i->clk[icl] = GSL_MAX(atm_i->clk[icl], 0);
      atm_i->sfz = GSL_MAX(atm_i->sfz, 0);
      atm_i->sfp = GSL_MAX(atm_i->sfp, 0);
      atm_i->sft = GSL_MIN(GSL_MAX(atm_i->sft, 100), 400);
      for (isf = 0; isf < ctl->nsf; isf++)
        atm_i->sfeps[isf] = GSL_MIN(GSL_MAX(atm_i->sfeps[isf], 0), 1);

      /* Forward calculation... */
      formod(ctl, atm_i, obs_i);
      obs2y(ctl, obs_i, y_i, NULL, NULL);

      /* Determine dx = x_i - x_a and dy = y - F(x_i) ... */
      gsl_vector_memcpy(dx, x_i);
      gsl_vector_sub(dx, x_a);
      gsl_vector_memcpy(dy, y_m);
      gsl_vector_sub(dy, y_i);

      /* Compute cost function... */
      chisq = cost_function(dx, dy, s_a_inv, sig_eps_inv);

      /* Modify Levenberg-Marquardt parameter... */
      if (chisq > chisq_old) {
        lmpar *= 10;
        gsl_vector_sub(x_i, x_step);
      } else {
        lmpar /= 10;
        break;
      }
    }

    /* Write info... */
    LOG(1, "it= %d / chi^2/m= %g", it, chisq);

    /* Write to cost function file... */
    fprintf(out, "%d %g %d %d\n", it, chisq, (int) m, (int) n);

    /* Get normalized step size in state space... */
    gsl_blas_ddot(x_step, b, &disq);
    disq /= (double) n;

    /* Convergence test... */
    if ((it == 1 || it % ret->kernel_recomp == 0) && disq < ret->conv_dmin)
      break;
  }

  /* Close cost function file... */
```

```
fclose(out);

/* Store results... */
write_atm(ret->dir, "atm_final.tab", ctl, atm_i);
write_obs(ret->dir, "obs_final.tab", ctl, obs_i);
write_matrix(ret->dir, "matrix_kernel.tab", ctl, k_i,
             atm_i, obs_i, "y", "x", "r");

/* ------------------------------------------------------------
   Analysis of retrieval results...
   ------------------------------------------------------------ */

/* Check if error analysis is requested... */
if (ret->err_ana) {

  /* Allocate... */
  auxnm = gsl_matrix_alloc(n, m);
  corr = gsl_matrix_alloc(n, n);
  gain = gsl_matrix_alloc(n, m);

  /* Compute inverse retrieval covariance...
     cov^{-1} = S_a^{-1} + K_i^T * S_eps^{-1} * K_i */
  matrix_product(k_i, sig_eps_inv, 1, cov);
  gsl_matrix_add(cov, s_a_inv);

  /* Compute retrieval covariance... */
  matrix_invert(cov);
  write_matrix(ret->dir, "matrix_cov_ret.tab", ctl, cov,
               atm_i, obs_i, "x", "x", "r");
  write_stddev("total", ret, ctl, atm_i, cov);

  /* Compute correlation matrix... */
  for (i = 0; i < n; i++)
    for (j = 0; j < n; j++)
      gsl_matrix_set(corr, i, j, gsl_matrix_get(cov, i, j)
                     / sqrt(gsl_matrix_get(cov, i, i))
                     / sqrt(gsl_matrix_get(cov, j, j)));
  write_matrix(ret->dir, "matrix_corr.tab", ctl, corr,
               atm_i, obs_i, "x", "x", "r");

  /* Compute gain matrix...
     G = cov * K^T * S_eps^{-1} */
  for (i = 0; i < n; i++)
    for (j = 0; j < m; j++)
      gsl_matrix_set(auxnm, i, j, gsl_matrix_get(k_i, j, i)
                     * POW2(gsl_vector_get(sig_eps_inv, j)));
  gsl_blas_dgemm(CblasNoTrans, CblasNoTrans, 1.0, cov, auxnm, 0.0, gain);
  write_matrix(ret->dir, "matrix_gain.tab", ctl, gain,
               atm_i, obs_i, "x", "y", "c");

  /* Compute retrieval error due to noise... */
  matrix_product(gain, sig_noise, 2, a);
  write_stddev("noise", ret, ctl, atm_i, a);

  /* Compute retrieval error  due to forward model errors... */
  matrix_product(gain, sig_formod, 2, a);
  write_stddev("formod", ret, ctl, atm_i, a);

  /* Compute averaging kernel matrix
     A = G * K ... */
  gsl_blas_dgemm(CblasNoTrans, CblasNoTrans, 1.0, gain, k_i, 0.0, a);
  write_matrix(ret->dir, "matrix_avk.tab", ctl, a,
               atm_i, obs_i, "x", "x", "r");

  /* Analyze averaging kernel matrix... */
  analyze_avk(ret, ctl, atm_i, iqa, ipa, a);

  /* Free... */
  gsl_matrix_free(auxnm);
  gsl_matrix_free(corr);
  gsl_matrix_free(gain);
}

/* ------------------------------------------------------------
   Finalize...
   ------------------------------------------------------------ */

gsl_matrix_free(a);
gsl_matrix_free(cov);
gsl_matrix_free(k_i);
gsl_matrix_free(s_a_inv);

gsl_vector_free(b);
gsl_vector_free(dx);
gsl_vector_free(dy);
gsl_vector_free(sig_eps_inv);
gsl_vector_free(sig_formod);
```

```
  gsl_vector_free(sig_noise);
  gsl_vector_free(x_a);
  gsl_vector_free(x_i);
  gsl_vector_free(x_step);
  gsl_vector_free(y_aux);
  gsl_vector_free(y_i);
  gsl_vector_free(y_m);
}

/*****************************************************************************/

void read_ret(
  int argc,
  char *argv[],
  ctl_t * ctl,
  ret_t * ret) {

  /* Iteration control... */
  ret->kernel_recomp =
    (int) scan_ctl(argc, argv, "KERNEL_RECOMP", -1, "3", NULL);
  ret->conv_itmax = (int) scan_ctl(argc, argv, "CONV_ITMAX", -1, "30", NULL);
  ret->conv_dmin = scan_ctl(argc, argv, "CONV_DMIN", -1, "0.1", NULL);

  /* Error analysis... */
  ret->err_ana = (int) scan_ctl(argc, argv, "ERR_ANA", -1, "1", NULL);

  for (int id = 0; id < ctl->nd; id++)
    ret->err_formod[id] = scan_ctl(argc, argv, "ERR_FORMOD", id, "0", NULL);

  for (int id = 0; id < ctl->nd; id++)
    ret->err_noise[id] = scan_ctl(argc, argv, "ERR_NOISE", id, "0", NULL);

  ret->err_press = scan_ctl(argc, argv, "ERR_PRESS", -1, "0", NULL);
  ret->err_press_cz = scan_ctl(argc, argv, "ERR_PRESS_CZ", -1, "-999", NULL);
  ret->err_press_ch = scan_ctl(argc, argv, "ERR_PRESS_CH", -1, "-999", NULL);

  ret->err_temp = scan_ctl(argc, argv, "ERR_TEMP", -1, "0", NULL);
  ret->err_temp_cz = scan_ctl(argc, argv, "ERR_TEMP_CZ", -1, "-999", NULL);
  ret->err_temp_ch = scan_ctl(argc, argv, "ERR_TEMP_CH", -1, "-999", NULL);

  for (int ig = 0; ig < ctl->ng; ig++) {
    ret->err_q[ig] = scan_ctl(argc, argv, "ERR_Q", ig, "0", NULL);
    ret->err_q_cz[ig] = scan_ctl(argc, argv, "ERR_Q_CZ", ig, "-999", NULL);
    ret->err_q_ch[ig] = scan_ctl(argc, argv, "ERR_Q_CH", ig, "-999", NULL);
  }

  for (int iw = 0; iw < ctl->nw; iw++) {
    ret->err_k[iw] = scan_ctl(argc, argv, "ERR_K", iw, "0", NULL);
    ret->err_k_cz[iw] = scan_ctl(argc, argv, "ERR_K_CZ", iw, "-999", NULL);
    ret->err_k_ch[iw] = scan_ctl(argc, argv, "ERR_K_CH", iw, "-999", NULL);
  }

  ret->err_clz = scan_ctl(argc, argv, "ERR_CLZ", -1, "0", NULL);
  ret->err_cldz = scan_ctl(argc, argv, "ERR_CLDZ", -1, "0", NULL);
  for (int icl = 0; icl < ctl->ncl; icl++)
    ret->err_clk[icl] = scan_ctl(argc, argv, "ERR_CLK", icl, "0", NULL);

  ret->err_sfz = scan_ctl(argc, argv, "ERR_SFZ", -1, "0", NULL);
  ret->err_sfp = scan_ctl(argc, argv, "ERR_SFP", -1, "0", NULL);
  ret->err_sft = scan_ctl(argc, argv, "ERR_SFT", -1, "0", NULL);
  for (int isf = 0; isf < ctl->nsf; isf++)
    ret->err_sfeps[isf] = scan_ctl(argc, argv, "ERR_SFEPS", isf, "0", NULL);
}

/*****************************************************************************/

void set_cov_apr(
  ret_t * ret,
  ctl_t * ctl,
  atm_t * atm,
  int *iqa,
  int *ipa,
  gsl_matrix * s_a) {

  gsl_vector *x_a;

  double x0[3], x1[3];

  /* Get sizes... */
  size_t n = s_a->size1;

  /* Allocate... */
  x_a = gsl_vector_alloc(n);

  /* Get sigma vector... */
  atm2x(ctl, atm, x_a, NULL, NULL);
  for (size_t i = 0; i < n; i++) {
```

```
    if (iqa[i] == IDXP)
      gsl_vector_set(x_a, i, ret->err_press / 100 * gsl_vector_get(x_a, i));
    if (iqa[i] == IDXT)
      gsl_vector_set(x_a, i, ret->err_temp);
    for (int ig = 0; ig < ctl->ng; ig++)
      if (iqa[i] == IDXQ(ig))
        gsl_vector_set(x_a, i, ret->err_q[ig] / 100 * gsl_vector_get(x_a, i));
    for (int iw = 0; iw < ctl->nw; iw++)
      if (iqa[i] == IDXK(iw))
        gsl_vector_set(x_a, i, ret->err_k[iw]);
    if (iqa[i] == IDXCLZ)
      gsl_vector_set(x_a, i, ret->err_clz);
    if (iqa[i] == IDXCLDZ)
      gsl_vector_set(x_a, i, ret->err_cldz);
    for (int icl = 0; icl < ctl->ncl; icl++)
      if (iqa[i] == IDXCLK(icl))
        gsl_vector_set(x_a, i, ret->err_clk[icl]);
    if (iqa[i] == IDXSFZ)
      gsl_vector_set(x_a, i, ret->err_sfz);
    if (iqa[i] == IDXSFP)
      gsl_vector_set(x_a, i, ret->err_sfp);
    if (iqa[i] == IDXSFT)
      gsl_vector_set(x_a, i, ret->err_sft);
    for (int isf = 0; isf < ctl->nsf; isf++)
      if (iqa[i] == IDXSFEPS(isf))
        gsl_vector_set(x_a, i, ret->err_sfeps[isf]);
  }

  /* Check standard deviations... */
  for (size_t i = 0; i < n; i++)
    if (POW2(gsl_vector_get(x_a, i)) <= 0)
      ERRMSG("Check a priori data (zero standard deviation)!");

  /* Initialize diagonal covariance... */
  gsl_matrix_set_zero(s_a);
  for (size_t i = 0; i < n; i++)
    gsl_matrix_set(s_a, i, i, POW2(gsl_vector_get(x_a, i)));

  /* Loop over matrix elements... */
  for (size_t i = 0; i < n; i++)
    for (size_t j = 0; j < n; j++)
      if (i != j && iqa[i] == iqa[j]) {

        /* Initialize... */
        double cz = 0;
        double ch = 0;

        /* Set correlation lengths for pressure... */
        if (iqa[i] == IDXP) {
          cz = ret->err_press_cz;
          ch = ret->err_press_ch;
        }

        /* Set correlation lengths for temperature... */
        if (iqa[i] == IDXT) {
          cz = ret->err_temp_cz;
          ch = ret->err_temp_ch;
        }

        /* Set correlation lengths for volume mixing ratios... */
        for (int ig = 0; ig < ctl->ng; ig++)
          if (iqa[i] == IDXQ(ig)) {
            cz = ret->err_q_cz[ig];
            ch = ret->err_q_ch[ig];
          }

        /* Set correlation lengths for extinction... */
        for (int iw = 0; iw < ctl->nw; iw++)
          if (iqa[i] == IDXK(iw)) {
            cz = ret->err_k_cz[iw];
            ch = ret->err_k_ch[iw];
          }

        /* Compute correlations... */
        if (cz > 0 && ch > 0) {

          /* Get Cartesian coordinates... */
          geo2cart(0, atm->lon[ipa[i]], atm->lat[ipa[i]], x0);
          geo2cart(0, atm->lon[ipa[j]], atm->lat[ipa[j]], x1);

          /* Compute correlations... */
          double rho =
            exp(-DIST(x0, x1) / ch -
                fabs(atm->z[ipa[i]] - atm->z[ipa[j]]) / cz);

          /* Set covariance... */
          gsl_matrix_set(s_a, i, j, gsl_vector_get(x_a, i)
```

```
                          * gsl_vector_get(x_a, j) * rho);
        }
      }

  /* Free... */
  gsl_vector_free(x_a);
}

/*****************************************************************************/

void set_cov_meas(
  ret_t * ret,
  ctl_t * ctl,
  obs_t * obs,
  gsl_vector * sig_noise,
  gsl_vector * sig_formod,
  gsl_vector * sig_eps_inv) {

  static obs_t obs_err;

  /* Get size... */
  size_t m = sig_eps_inv->size;

  /* Noise error (always considered in retrieval fit)... */
  copy_obs(ctl, &obs_err, obs, 1);
  for (int ir = 0; ir < obs_err.nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      obs_err.rad[id][ir]
        = (gsl_finite(obs->rad[id][ir]) ? ret->err_noise[id] : GSL_NAN);
  obs2y(ctl, &obs_err, sig_noise, NULL, NULL);

  /* Forward model error (always considered in retrieval fit)... */
  copy_obs(ctl, &obs_err, obs, 1);
  for (int ir = 0; ir < obs_err.nr; ir++)
    for (int id = 0; id < ctl->nd; id++)
      obs_err.rad[id][ir]
        = fabs(ret->err_formod[id] / 100 * obs->rad[id][ir]);
  obs2y(ctl, &obs_err, sig_formod, NULL, NULL);

  /* Total error... */
  for (size_t i = 0; i < m; i++)
    gsl_vector_set(sig_eps_inv, i, 1 / sqrt(POW2(gsl_vector_get(sig_noise, i))
                                            +
                                            POW2(gsl_vector_get
                                                 (sig_formod, i))));

  /* Check standard deviations... */
  for (size_t i = 0; i < m; i++)
    if (gsl_vector_get(sig_eps_inv, i) <= 0)
      ERRMSG("Check measurement errors (zero standard deviation)!");
}

/*****************************************************************************/

void write_stddev(
  const char *quantity,
  ret_t * ret,
  ctl_t * ctl,
  atm_t * atm,
  gsl_matrix * s) {

  static atm_t atm_aux;

  gsl_vector *x_aux;

  char filename[LEN];

  /* Get sizes... */
  size_t n = s->size1;

  /* Allocate... */
  x_aux = gsl_vector_alloc(n);

  /* Compute standard deviation... */
  for (size_t i = 0; i < n; i++)
    gsl_vector_set(x_aux, i, sqrt(gsl_matrix_get(s, i, i)));

  /* Write to disk... */
  copy_atm(ctl, &atm_aux, atm, 1);
  x2atm(ctl, x_aux, &atm_aux);
  sprintf(filename, "atm_err_%s.tab", quantity);
  write_atm(ret->dir, filename, ctl, &atm_aux);

  /* Free... */
  gsl_vector_free(x_aux);
}
```

5.35 tblfmt.c File Reference

Convert look-up table file format.

```
#include "jurassic.h"
```

Functions

- int main (int argc, char ∗argv[ ])

5.35.1 Detailed Description

Convert look-up table file format.

Definition in file tblfmt.c.

5.35.2 Function Documentation

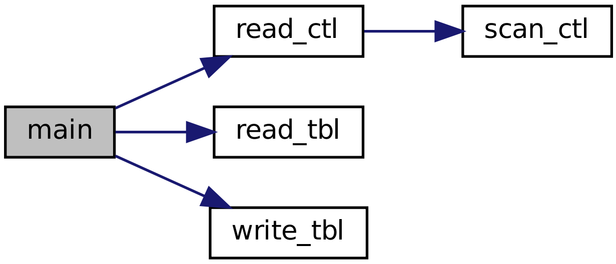
5.35.2.1 main()

```
int main (
    int argc,
    char ∗ argv[ ] )
```

Definition at line 27 of file tblfmt.c.

```
                  {

  ctl_t ctl;

  tbl_t *tbl;

  /* Check arguments... */
  if (argc < 6)
    ERRMSG("Give parameters: <ctl> <tblbase_in> <tblfmt_in>"
           " <tblbase_out> <tblfmt_out>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Allocate... */
  ALLOC(tbl, tbl_t, 1);

  /* Read tables... */
  sprintf(ctl.tblbase, "%s", argv[2]);
  ctl.tblfmt = atoi(argv[3]);
  read_tbl(&ctl, tbl);

  /* Write tables... */
  sprintf(ctl.tblbase, "%s", argv[4]);
  ctl.tblfmt = atoi(argv[5]);
  write_tbl(&ctl, tbl);

  /* Free... */
  free(tbl);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.36 tblfmt.c

```c
/*
  This file is part of JURASSIC.

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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2013-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  ctl_t ctl;

  tbl_t *tbl;

  /* Check arguments... */
  if (argc < 6)
    ERRMSG("Give parameters: <ctl> <tblbase_in> <tblfmt_in>"
           " <tblbase_out> <tblfmt_out>");

  /* Read control parameters... */
  read_ctl(argc, argv, &ctl);

  /* Allocate... */
  ALLOC(tbl, tbl_t, 1);

  /* Read tables... */
  sprintf(ctl.tblbase, "%s", argv[2]);
  ctl.tblfmt = atoi(argv[3]);
  read_tbl(&ctl, tbl);

  /* Write tables... */
  sprintf(ctl.tblbase, "%s", argv[4]);
  ctl.tblfmt = atoi(argv[5]);
  write_tbl(&ctl, tbl);

  /* Free... */
  free(tbl);

  return EXIT_SUCCESS;
}
```

5.37 tblgen.c File Reference

Prepapre look-up tables from monochromatic absorption spectra.

```
#include "jurassic.h"
```

Macros

- #define MAXNF 10000
- #define MAXNPTS 10000000
- #define MAXLINE 100000

Functions

- int main (int argc, char *argv[ ])

5.37.1 Detailed Description

Prepapre look-up tables from monochromatic absorption spectra.

Definition in file tblgen.c.

5.37.2 Macro Definition Documentation

5.37.2.1 MAXNF `#define MAXNF 10000`

Definition at line 32 of file tblgen.c.

5.37.2.2 MAXNPTS `#define MAXNPTS 10000000`

Definition at line 35 of file tblgen.c.

5.37.2.3 MAXLINE `#define MAXLINE 100000`

Definition at line 38 of file tblgen.c.

5.37.3 Function Documentation

5.37.3.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Definition at line 44 of file tblgen.c.

```
                {

FILE *in;

static char line[MAXLINE], *tok;

static double dnu, abs[MAXNPTS], epsold, f, filt[MAXNF],
  nu, nu0, nu1, nuf[MAXNF], press, r0, temp, u;

static int i, i0, idx, nf, npts;

/* Read command line arguments... */
if (argc != 5)
  ERRMSG("Give parameters: <press> <temp> <spec> <filter>");
sscanf(argv[1], "%lg", &press);
sscanf(argv[2], "%lg", &temp);

/* Compute column density [molec/cm^2] (1 km path length, 1 ppmv)... */
u = 1e-6 * press * 100 / (1.380658e-23 * temp) * 1000 / 1e4;

/* Read filter function... */
if (!(in = fopen(argv[4], "r")))
  ERRMSG("Cannot open filter file!");
while (fgets(line, MAXLINE, in))
  if (sscanf(line, "%lg %lg", &nuf[nf], &filt[nf]) == 2)
    if (++nf >= MAXNF)
      ERRMSG("Too many points in filter function");
fclose(in);

/* Read spectrum... */
if (!(in = fopen(argv[3], "r")))
  ERRMSG("Cannot open spectrum!");
if (!fgets(line, MAXLINE, in))
  ERRMSG("Error while reading spectrum!");
if (!fgets(line, MAXLINE, in))
  ERRMSG("Error while reading spectrum!");
if (!fgets(line, MAXLINE, in))
  ERRMSG("Error while reading spectrum!");
if (!fgets(line, MAXLINE, in))
  ERRMSG("Error while reading spectrum!");
sscanf(line, "%d %lg %lg %lg", &npts, &nu0, &dnu, &nu1);
if (npts > MAXNPTS)
  ERRMSG("Too many points in optical depth spectrum!");
i = 0;
while (fgets(line, MAXLINE, in)) {
  if ((tok = strtok(line, " \t\n")) != NULL) {
    sscanf(tok, "%lg", &abs[i]);
    abs[i] /= u;
    i++;
  }
  while ((tok = strtok(NULL, " \t\n")) != NULL) {
    sscanf(tok, "%lg", &abs[i]);
    abs[i] /= u;
    i++;
  }
}
fclose(in);

/* Set grid spacing... */
dnu = (nu1 - nu0) / ((double) npts - 1.0);
r0 = (nuf[0] - nu0) / (nu1 - nu0) * (double) npts;
i0 = (int) r0;

/* Loop over column densities... */
for (u = 1.0; u <= 1e30; u *= 1.122) {

  /* Integrate... */
  double epssum = 0, fsum = 0;
  for (i = i0; i < npts; i++) {
    nu = nu0 + dnu * (double) i;
    if (nu < nuf[0])
      continue;
    else if (nu > nuf[nf - 1])
      break;
    else {
      if (nu < nuf[idx] || nu > nuf[idx + 1])
        idx = locate_irr(nuf, nf, nu);
      f = LIN(nuf[idx], filt[idx], nuf[idx + 1], filt[idx + 1], nu);
      fsum += f;
      epssum += f * exp(-abs[i] * u);
```

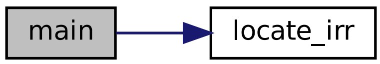
```
    }
  }
  epssum = 1 - epssum / fsum;

  /* Write output... */
  if (epssum >= 1e-6 && epssum <= 0.999999 && epssum > epsold)
    printf("%g %g %g %g\n", press, temp, u, epssum);
  epsold = epssum;

  /* Check for termination... */
  if (epssum > 0.999999)
    return EXIT_SUCCESS;
}

return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.38 tblgen.c

```
/*
  This file is part of JURASSIC.

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  it under the terms of the GNU General Public License as published by
  the Free Software Foundation, either version 3 of the License, or
  (at your option) any later version.

  JURASSIC is distributed in the hope that it will be useful,
  but WITHOUT ANY WARRANTY; without even the implied warranty of
  MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
  GNU General Public License for more details.

  You should have received a copy of the GNU General Public License
  along with JURASSIC. If not, see <http://www.gnu.org/licenses/>.

  Copyright (C) 2003-2021 Forschungszentrum Juelich GmbH
*/

#include "jurassic.h"

/* ------------------------------------------------------------
   Dimensions...
   ------------------------------------------------------------ */

/* Maximum number of grid points for filter files: */
#define MAXNF 10000

/* Maximum number of grid points for spectra: */
#define MAXNPTS 10000000

/* Maximum line length: */
#define MAXLINE 100000

/* ------------------------------------------------------------
   Main...
   ------------------------------------------------------------ */

int main(
  int argc,
  char *argv[]) {

  FILE *in;

  static char line[MAXLINE], *tok;

  static double dnu, abs[MAXNPTS], epsold, f, filt[MAXNF],
```

```
    nu, nu0, nu1, nuf[MAXNF], press, r0, temp, u;

  static int i, i0, idx, nf, npts;

  /* Read command line arguments... */
  if (argc != 5)
    ERRMSG("Give parameters: <press> <temp> <spec> <filter>");
  sscanf(argv[1], "%lg", &press);
  sscanf(argv[2], "%lg", &temp);

  /* Compute column density [molec/cm^2] (1 km path length, 1 ppmv)... */
  u = 1e-6 * press * 100 / (1.380658e-23 * temp) * 1000 / 1e4;

  /* Read filter function... */
  if (!(in = fopen(argv[4], "r")))
    ERRMSG("Cannot open filter file!");
  while (fgets(line, MAXLINE, in))
    if (sscanf(line, "%lg %lg", &nuf[nf], &filt[nf]) == 2)
      if (++nf >= MAXNF)
        ERRMSG("Too many points in filter function");
  fclose(in);

  /* Read spectrum... */
  if (!(in = fopen(argv[3], "r")))
    ERRMSG("Cannot open spectrum!");
  if (!fgets(line, MAXLINE, in))
    ERRMSG("Error while reading spectrum!");
  if (!fgets(line, MAXLINE, in))
    ERRMSG("Error while reading spectrum!");
  if (!fgets(line, MAXLINE, in))
    ERRMSG("Error while reading spectrum!");
  if (!fgets(line, MAXLINE, in))
    ERRMSG("Error while reading spectrum!");
  sscanf(line, "%d %lg %lg %lg", &npts, &nu0, &dnu, &nu1);
  if (npts > MAXNPTS)
    ERRMSG("Too many points in optical depth spectrum!");
  i = 0;
  while (fgets(line, MAXLINE, in)) {
    if ((tok = strtok(line, " \t\n")) != NULL) {
      sscanf(tok, "%lg", &abs[i]);
      abs[i] /= u;
      i++;
    }
    while ((tok = strtok(NULL, " \t\n")) != NULL) {
      sscanf(tok, "%lg", &abs[i]);
      abs[i] /= u;
      i++;
    }
  }
  fclose(in);

  /* Set grid spacing... */
  dnu = (nu1 - nu0) / ((double) npts - 1.0);
  r0 = (nuf[0] - nu0) / (nu1 - nu0) * (double) npts;
  i0 = (int) r0;

  /* Loop over column densities... */
  for (u = 1.0; u <= 1e30; u *= 1.122) {

    /* Integrate... */
    double epssum = 0, fsum = 0;
    for (i = i0; i < npts; i++) {
      nu = nu0 + dnu * (double) i;
      if (nu < nuf[0])
        continue;
      else if (nu > nuf[nf - 1])
        break;
      else {
        if (nu < nuf[idx] || nu > nuf[idx + 1])
          idx = locate_irr(nuf, nf, nu);
        f = LIN(nuf[idx], filt[idx], nuf[idx + 1], filt[idx + 1], nu);
        fsum += f;
        epssum += f * exp(-abs[i] * u);
      }
    }
    epssum = 1 - epssum / fsum;

    /* Write output... */
    if (epssum >= 1e-6 && epssum <= 0.999999 && epssum > epsold)
      printf("%g %g %g %g\n", press, temp, u, epssum);
    epsold = epssum;

    /* Check for termination... */
    if (epssum > 0.999999)
      return EXIT_SUCCESS;
  }

```

```
  return EXIT_SUCCESS;
}
```

5.39 time2jsec.c File Reference

Convert date to Julian seconds.

`#include "jurassic.h"`

Functions

- int main (int argc, char ∗argv[ ])

5.39.1 Detailed Description

Convert date to Julian seconds.

Definition in file time2jsec.c.

5.39.2 Function Documentation

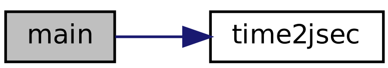
5.39.2.1 main()

```
int main (
    int argc,
    char * argv[ ] )
```

Definition at line 27 of file time2jsec.c.

```
                      {

  double jsec;

  /* Check arguments... */
  if (argc < 8)
    ERRMSG("Give parameters: <year> <mon> <day> <hour> <min> <sec> <remain>");

  /* Read arguments... */
  int year = atoi(argv[1]);
  int mon = atoi(argv[2]);
  int day = atoi(argv[3]);
  int hour = atoi(argv[4]);
  int min = atoi(argv[5]);
  int sec = atoi(argv[6]);
  double remain = atof(argv[7]);

  /* Convert... */
  time2jsec(year, mon, day, hour, min, sec, remain, &jsec);
  printf("%.2f\n", jsec);

  return EXIT_SUCCESS;
}
```

Here is the call graph for this function:



5.40 time2jsec.c

```
/*
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*/

#include "jurassic.h"

int main(
  int argc,
  char *argv[]) {

  double jsec;

  /* Check arguments... */
  if (argc < 8)
    ERRMSG("Give parameters: <year> <mon> <day> <hour> <min> <sec> <remain>");

  /* Read arguments... */
  int year = atoi(argv[1]);
  int mon = atoi(argv[2]);
  int day = atoi(argv[3]);
  int hour = atoi(argv[4]);
  int min = atoi(argv[5]);
  int sec = atoi(argv[6]);
  double remain = atof(argv[7]);

  /* Convert... */
  time2jsec(year, mon, day, hour, min, sec, remain, &jsec);
  printf("%.2f\n", jsec);

  return EXIT_SUCCESS;
}
```

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